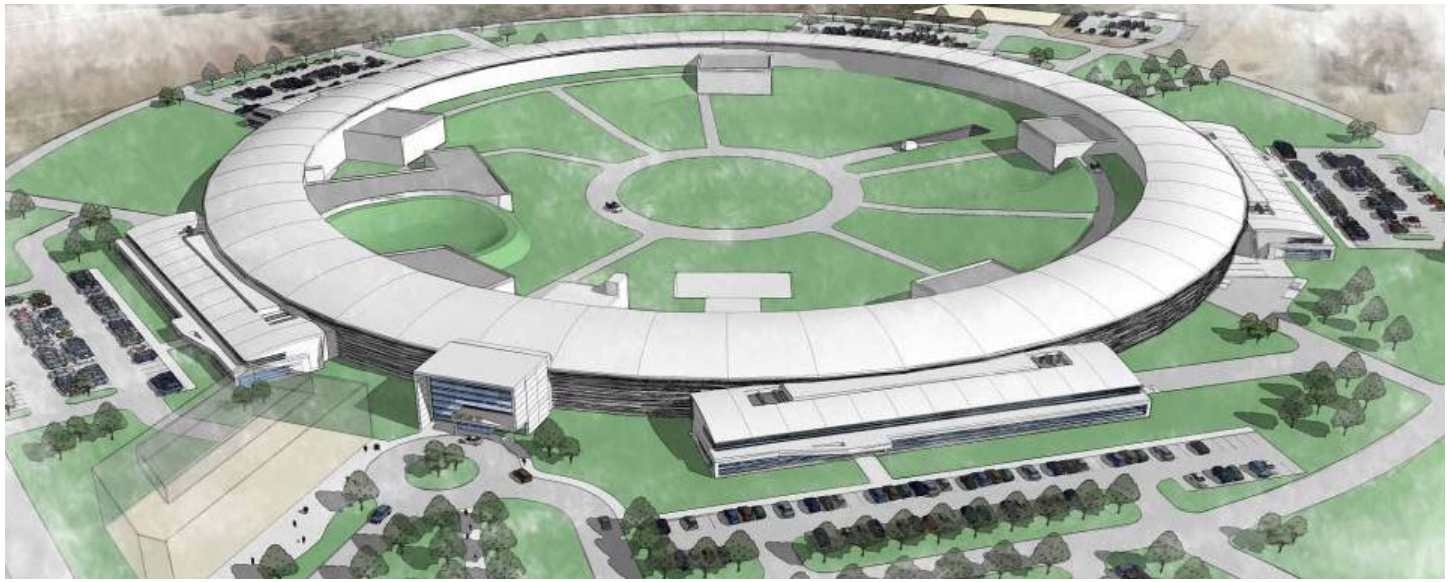
National Synchrotron Light Source II



Inelastic X-ray Scattering Beamline

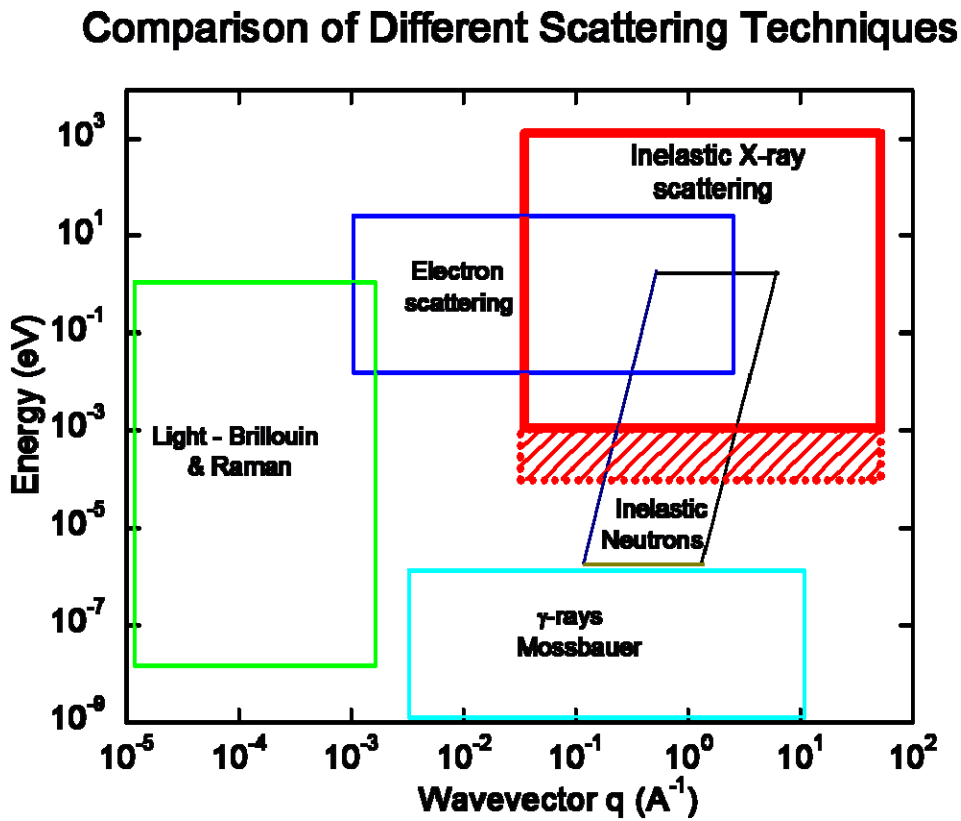
Yong Cai
October 4, 2007

Office of Science
U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY
BROOKHAVEN SCIENCE ASSOCIATES

Scientific Mission

- To develop advanced IXS instrumentation afforded by the high brightness and flux of NSLS-II that would enable IXS experiments at extremely high resolution of 0.1 meV at ~10 keV – *a key goal for NSLS-II.*



Bridging the gap between existing high and low frequency probes, and enabling new sciences

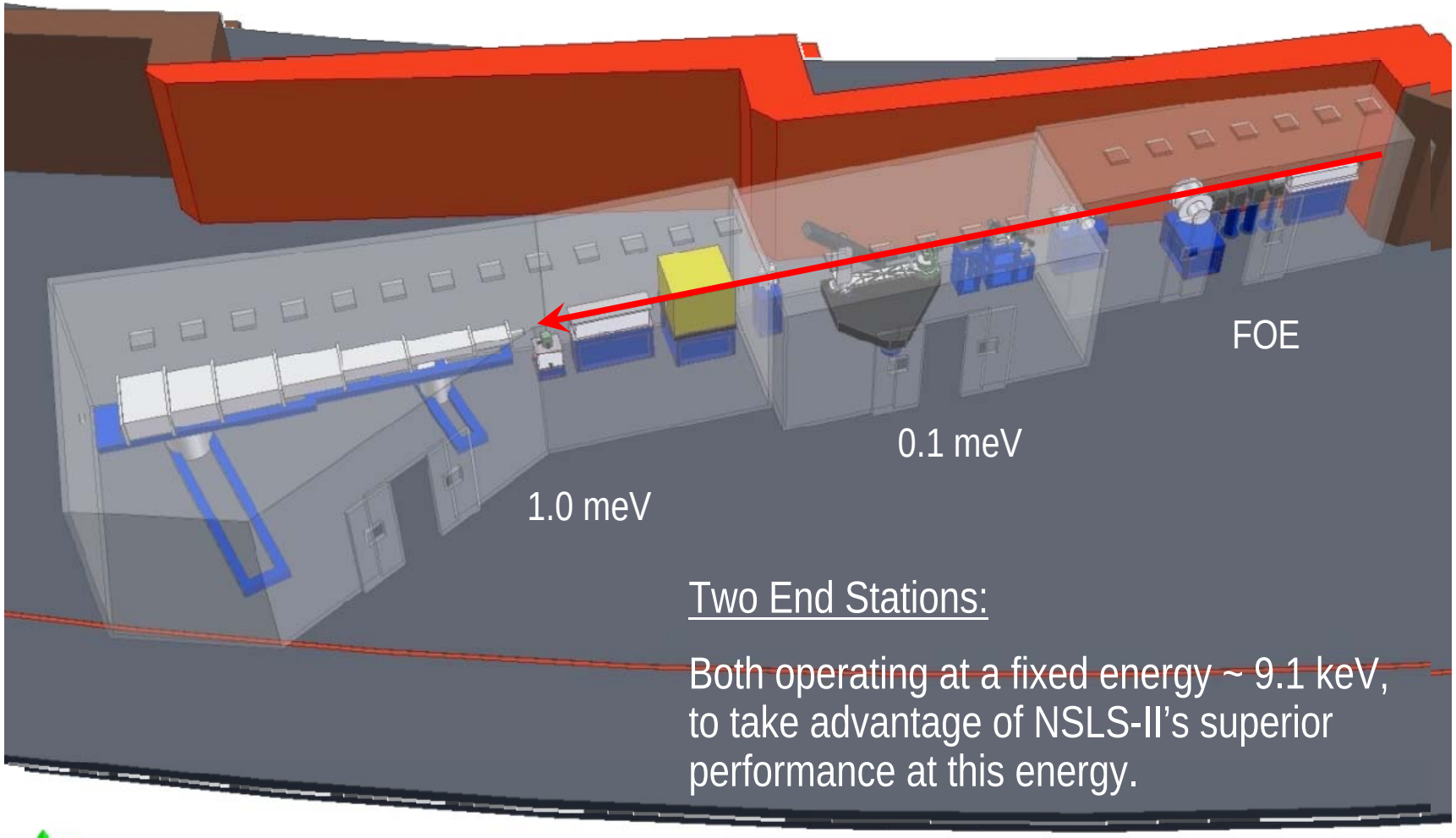
Scientific Mission

Based on CDR December 2006 and Conclusions drawn from July NSLS-II Workshop

- 0.1-meV resolution end station
  - Visco-elastic behaviors of disordered systems and fluids
  - New modes in complex fluids and confined systems
  - Collective modes in lipid membranes and other biological systems
- 1-meV resolution end station
  - Relaxation processes in disordered systems (glasses, fluids, polymers …)
  - Phonons in single crystals, surfaces, thin films, high pressure systems, small samples, strongly correlated systems …
- 10~50-meV resolution - *On a separate beamline dedicated for electronic excitations*
  - High flux experiments
  - X-ray Raman combined with small beam for small samples of nanoscale, high pressure, high fields, low and high T…
  - Resonant inelastic scattering
  - Experiments with low(er) energy resolution

Beamline Layout

Designed to cater for the 0.1-meV and 1-meV scientific mission



Two End Stations:

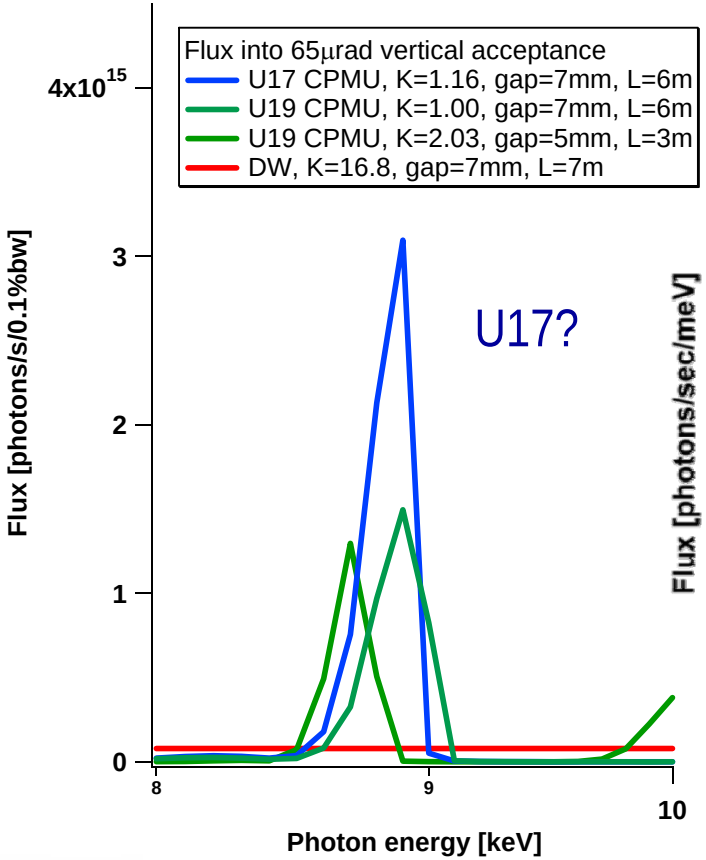
Both operating at a fixed energy ~ 9.1 keV, to take advantage of NSLS-II's superior performance at this energy.

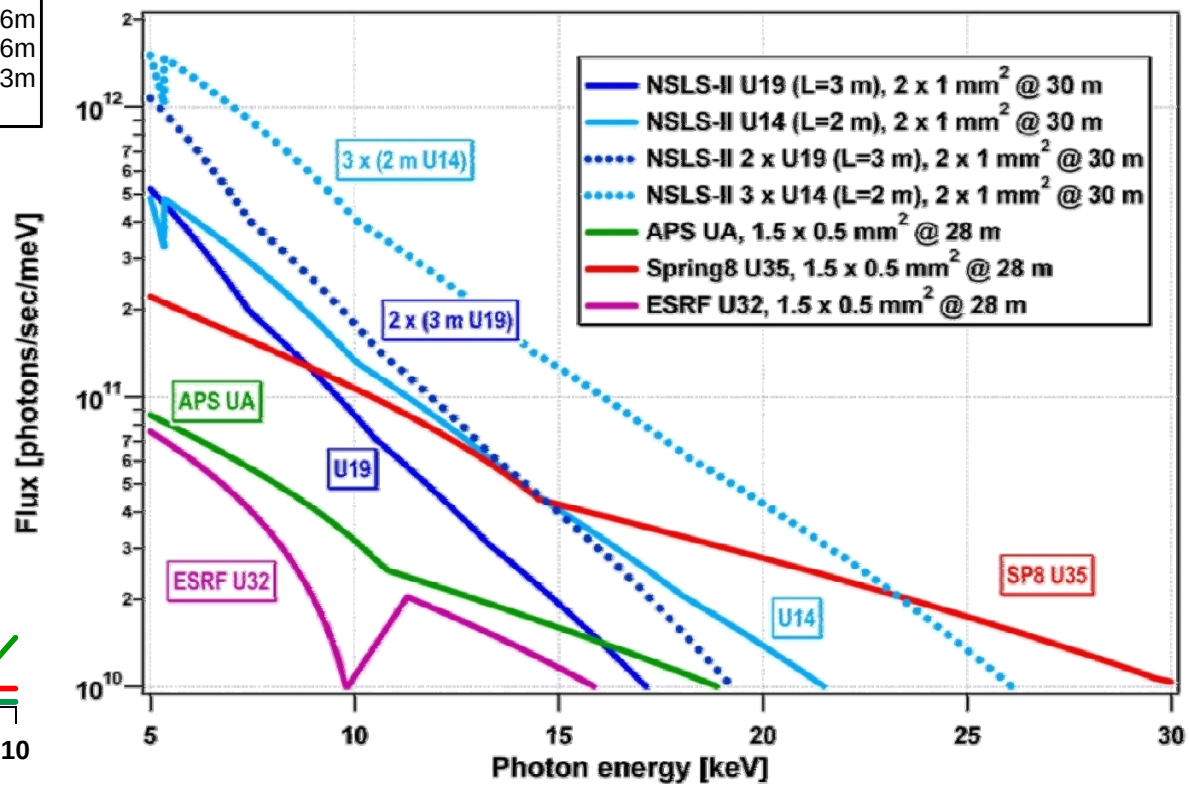
Requirements and Specifications

- Radiation Source
  - Should provide the highest possible flux at ~ 10 keV – photon hungry experiments
  - Should provide essential source size and divergence stability, vibration and thermal stability to achieve the 0.1-meV resolution (more later)
- Beamline and End Station Specifications
  - Primary beam energy at 9.1 keV, tunable over 7~12 keV for added flexibility
  - Energy resolution: up to 0.1 meV for 1st, and 1 meV for 2nd end station
  - Energy scan range: order of 100 meV, appropriate for the excitations to be studied
  - Momentum resolution: 0.01~0.04 Å^{-1} (10 mrad angular acceptance at 9.1keV)
  - Momentum scan range: up to 8 Å^{-1} (120° at 9.1 keV) to cover typical BZ sizes
  - Spot size: ≤ 5 μm (V) x 10 μm (H)
  - Flux: as much as possibly achievable optically
  - Sample environments: crystal alignment capability, handling of small samples of micrometer scale, high pressure, low and high temperature …, etc.

Insertion Device

- Candidates: U19 (CPMU), or U14 (SC) on a high-β straight (more later)
  Figure of Merit: Flux / meV – provide the highest possible flux at ~ 10 keV
  Future upgrade: 2xU19 / 3xU14 on a 9.3 m straight, candidate for an extended straight





High-β vs Low-β Straight

- Photon source size and divergence (horizontal emittance: 0.55 nm-rad)

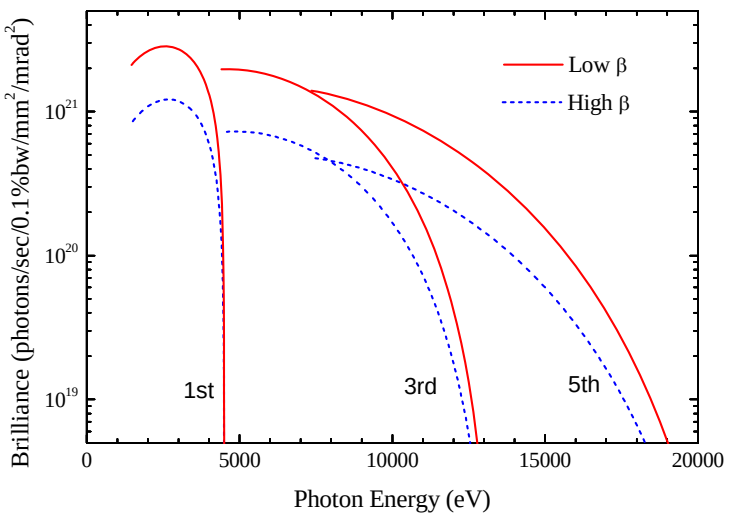
K	N	E, keV	Source size (σ), μm				Angular Divergence (σ), μrad			
			Low-β		High-β		Low-β		High-β	
			H	V	H	V	H	V	H	V
2.03	1	1.47	29.3	6.2	99.7	7.5	22.5	12.3	13.1	12.0
1.713	5	9.1	28.8	3.4	99.5	5.5	19.8	5.7	7.3	5.0
0.981	3	9.1	28.8	3.4	99.5	5.5	19.8	5.7	7.3	5.0

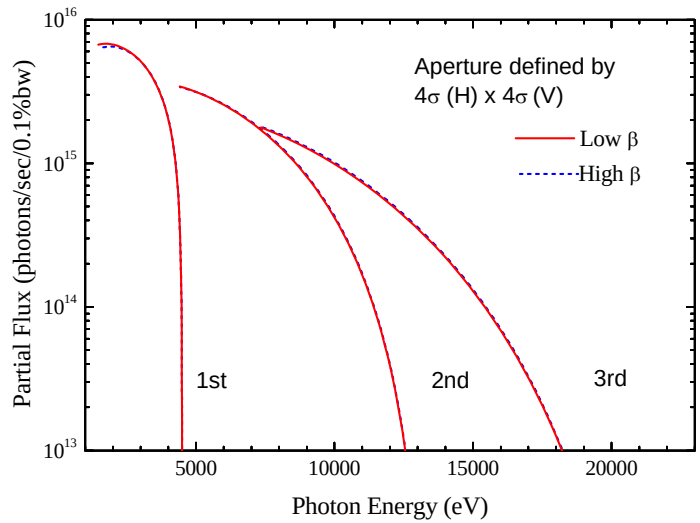
- Power and power density at 30m from the source (aperture: 4σ(H) x 4σ(V))

Distance, m	K	Low-β			High-β		
		Aperture (HxV),	Power density, W/mm^2	Power, W	Aperture (HxV),	Power density, W/mm^2	Power, W
30	1.713	79.2 x 22.8	72.8	118	29.2 x 20.0	72.9	38
30	0.981	79.2 x 22.8	40.1	65	29.2 x 20.0	40.4	21

High-β vs Low-β Straight

- The differences of a high-β compared to a low-β straight:
  Horiz. source size is ~3.5 times larger, whereas horiz. divergence is ~2.7 times smaller
- The consequences of moving from a low-β to a high-β straight:
  Horiz. beam size downstream and power on the first optics reduce by ~ a factor of 3
  Brightness reduced by ~ a factor of 2 at ~ 10 keV
  Flux delivered thru a 4σ(H) x 4σ(V) aperture remains essentially the same

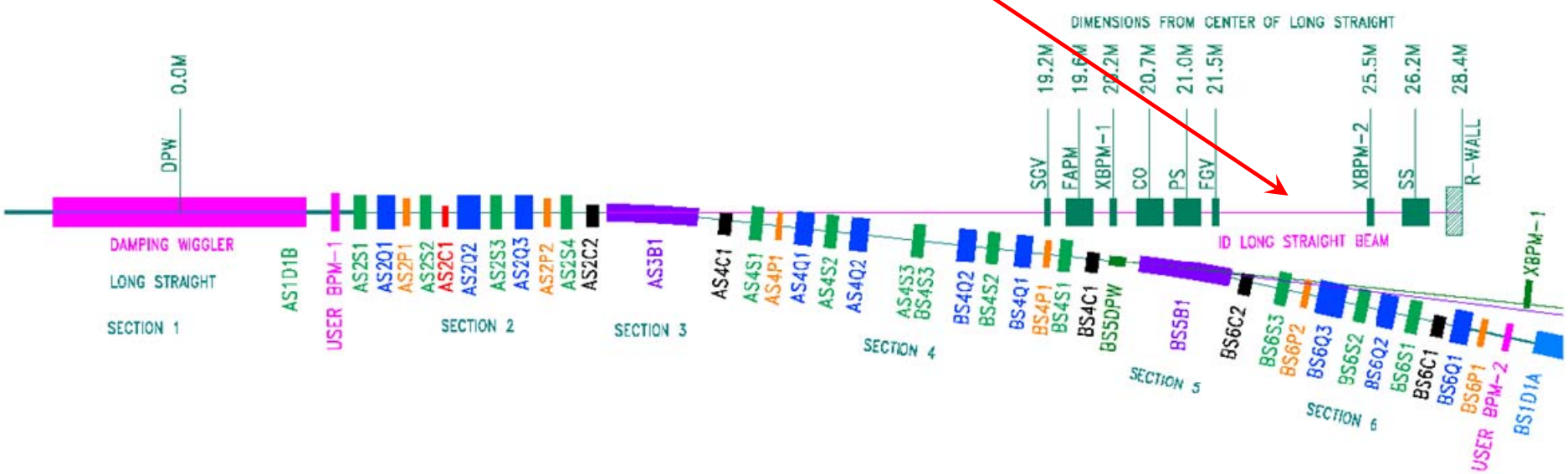




➢ A high-β straight seems a logical choice

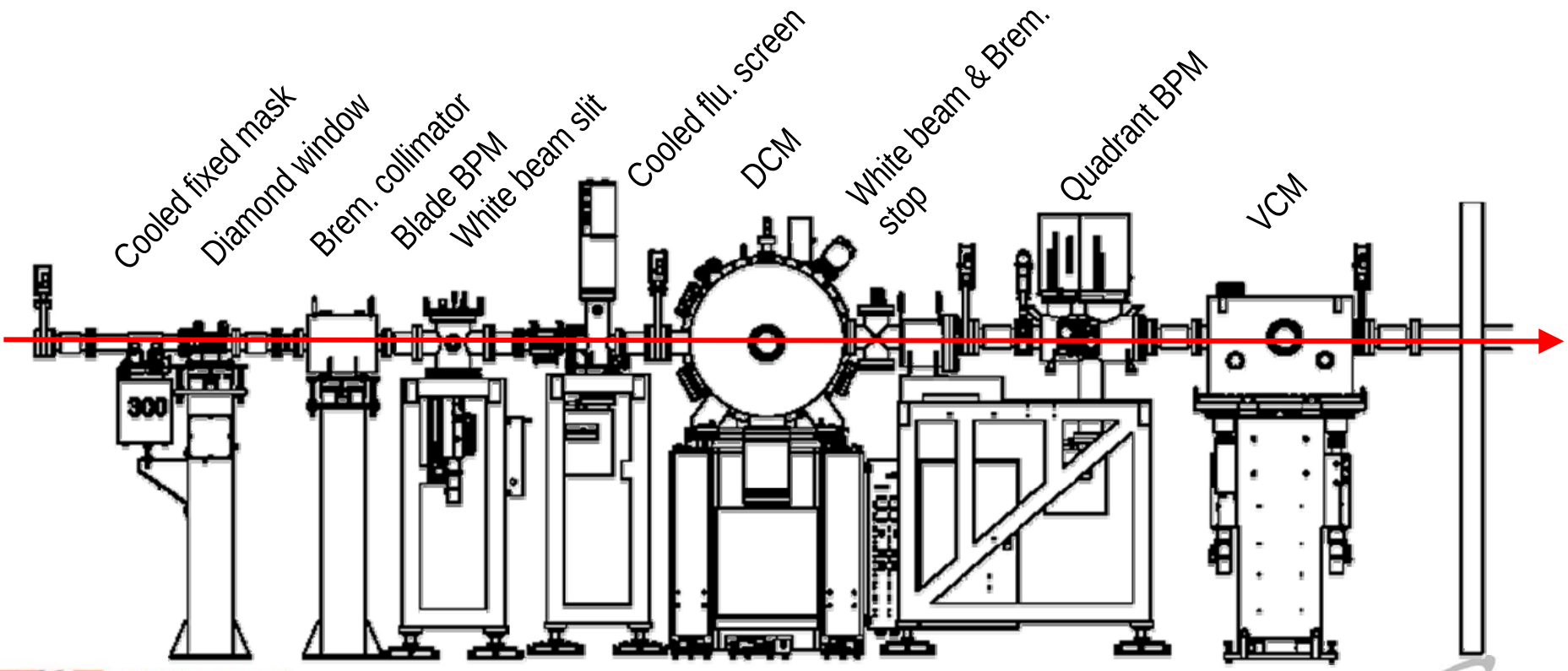
Front end Layout

- Standard front end for 9.3m long straights
- Aperture (fixed mask and white beam slit) defining a radiation fan of 4 σ (H) x 4 σ (V) transmitting ~ 96% total flux and cutting out majority of the heat power, currently planned to be part of the FOE components, could be relocated to the front end to save space for the beamline

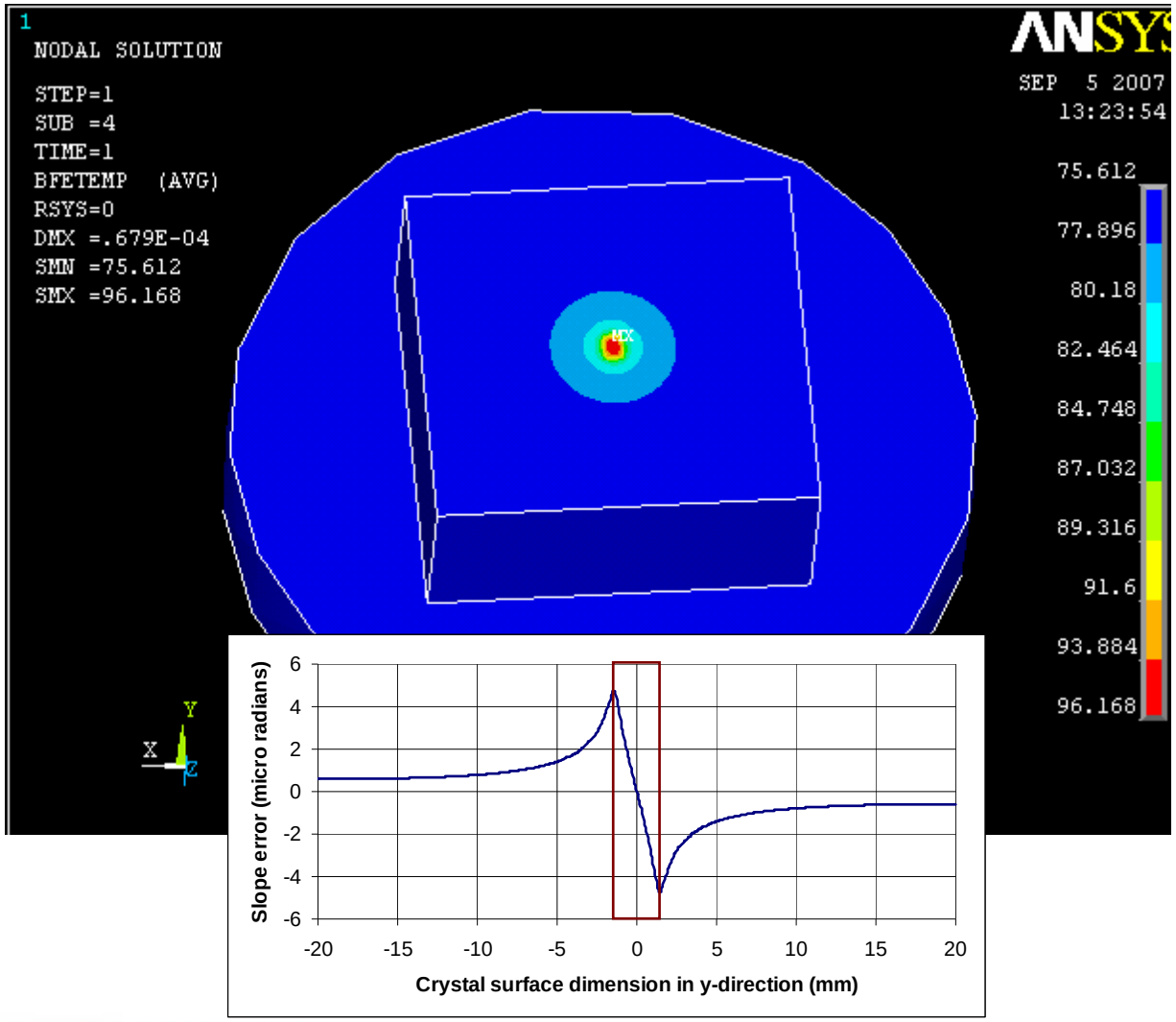


First Optics Enclosure (FOE)

- DCM: cryogenic cooled Si(111)
- Water cooled Diamond is less preferable due to the poor quality, mounting strain and small size of available crystals
- FEA analysis on first crystal of DCM shows that water-cooled Si is not an option



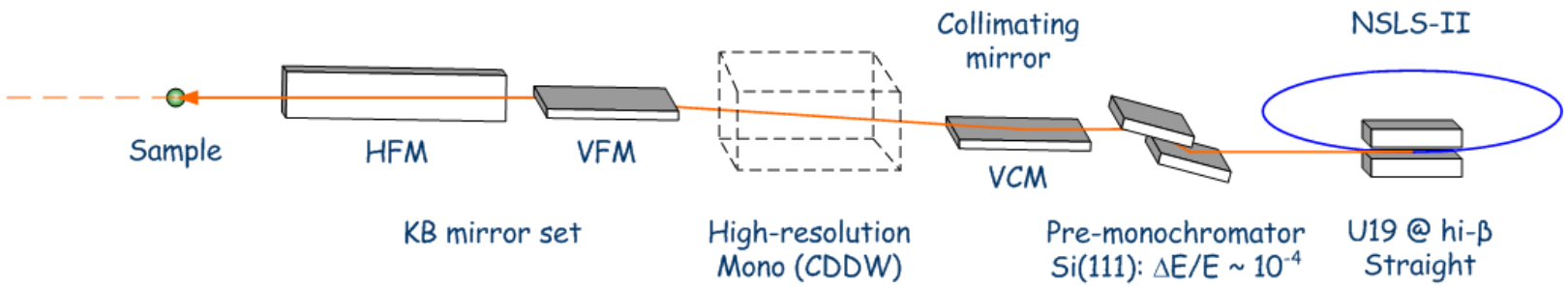
FEA Analysis of First Optics



Simulation of liquid nitrogen cooled Si crystal:

- 4 σ (H) x 4 σ (V) cone
- K = 1.717 (two U19)
- Low-beta at 0.55 nm-rad
- Power (filtered) 115 W
- Maximum temperature = 94 K
- Maximum thermal slope error in beam footprint = $\pm$4.6 µrad
- For high-beta, thermal effect would be less a problem due to the lower heat load.

Shadow Ray Tracing with FEA Results



Case	Model , LN2 cooled DCM (ε_x = 0.55nm-rad)	Spot size , μ m	Flux, phs/sec (No distortion)	Spot size, μ m	Flux, phs/sec (W/ distortion)
1	Lo-β , K=0.981, 1 x U19, 22W	2.0 x 1.8	1.50 x 10^{13}	2.1 x 2.1	1.49 x 10^{13}
2	Hi-β , K=0.981, 1 x U19, 7W	7.0 x 1.8	1.49 x 10^{13}	7.0 x 2.0	1.49 x 10^{13}
2a	Same as 2, but water cooled	7.0 x 1.8	1.49 x 10^{13}	16 x 7.4	1.51 x 10^{13}
3	Lo-β , K=1.714, 1 x U19, 71W	2.0 x 1.9	2.88 x 10^{13}	2.3 x 4.2	2.81 x 10^{13}
3a	Same as 3, but hot spot at 125K	2.0 x 1.9	2.88 x 10^{13}	2.1 x 0.5	2.92 x 10^{13}
3b	Same as 3, but 2 x U19, 115W	2.0 x 2.0	5.80 x 10^{13}	2.9 x 5.9	5.14 x 10^{13}
4	Hi-β , K=1.714, 1 x U19, 22W	7.1 x 1.9	2.81 x 10^{13}	7.0 x 3.4	2.79 x 10^{13}

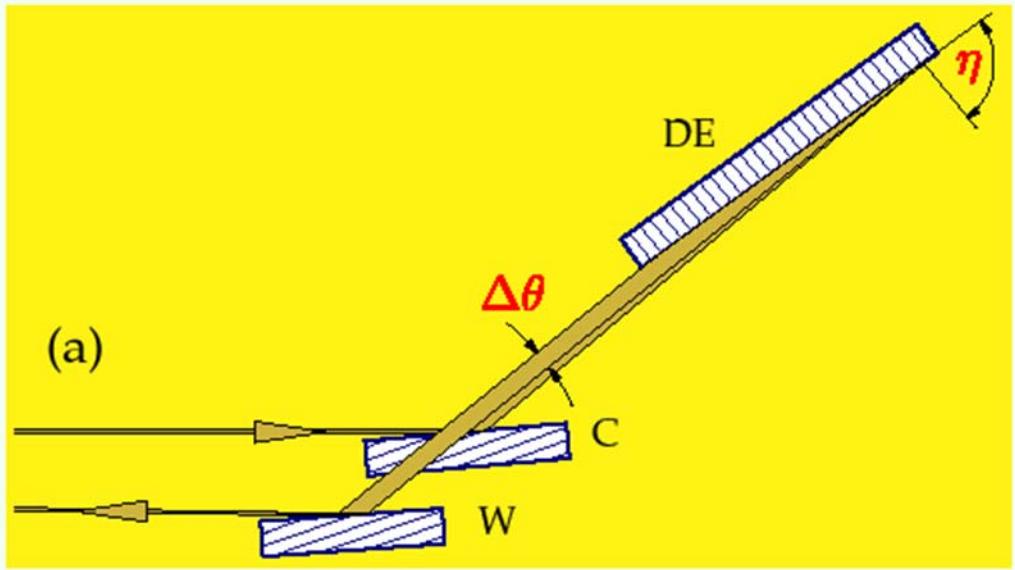
Angular Dispersive Monochromator

- Scheme for achieving 0.1 meV resolution at ~10 keV (Yu. Shvyd'ko)

$$\frac{\Delta E}{E} = \frac{\Delta\theta}{\tan\eta}$$

$$\frac{\Delta E}{E} = 10^{-6} - 10^{-8}$$

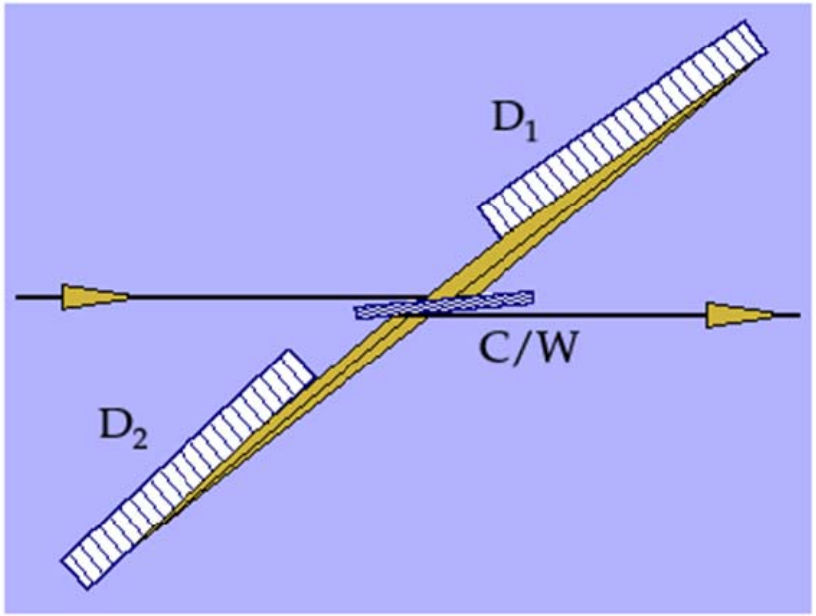
is feasible

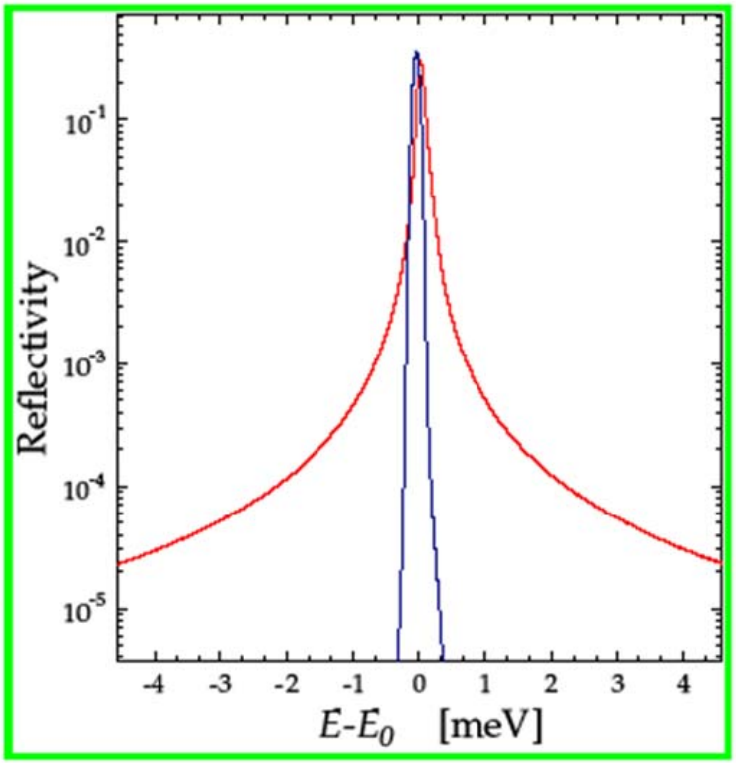


$$E = 10 \text{ keV} \Rightarrow \quad \Delta E = 10 - 0.1 \text{ meV}$$
$$E = 5 \text{ keV} \Rightarrow \quad \Delta E = 5 - 0.05 \text{ meV}$$

A prototype CDW monochromator achieving ΔE = 2.2 meV for 9.1keV photons has been demonstrated *(Shvyd'ko et al, PRL 97, 235502)*

In-line CDDW Monochromator





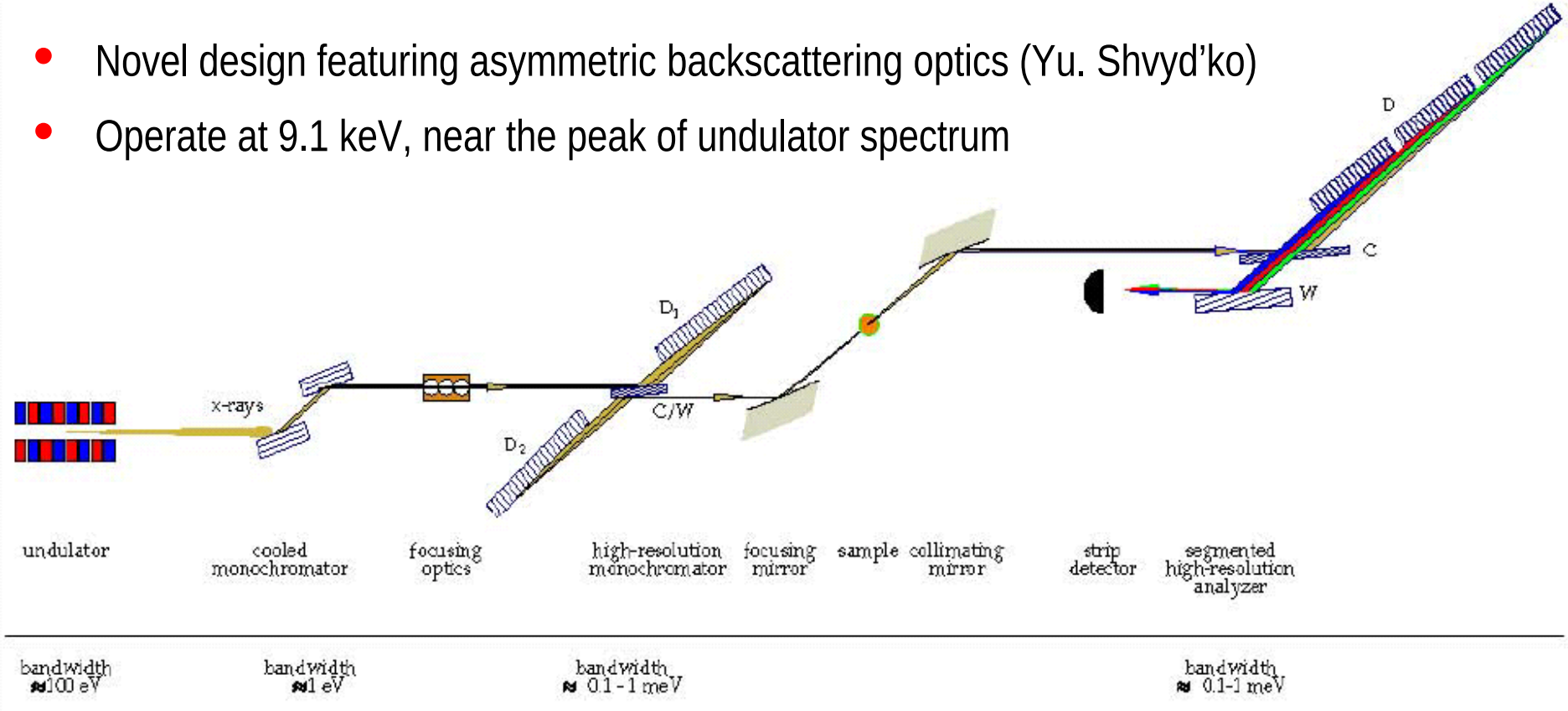
Adding one more dispersive element (D_2) makes it an in-line monochromator, and produces a symmetric resolution profile.

Angular-dispersive CDDW monochromator:
$E = 9.1315$ keV, $\Delta E = 0.1$ meV, D=Si(008)

Single-bounce backscattering monochromator:
$E = 31.02$ keV, $\Delta E = 0.1$ meV, Si(1 3 27).

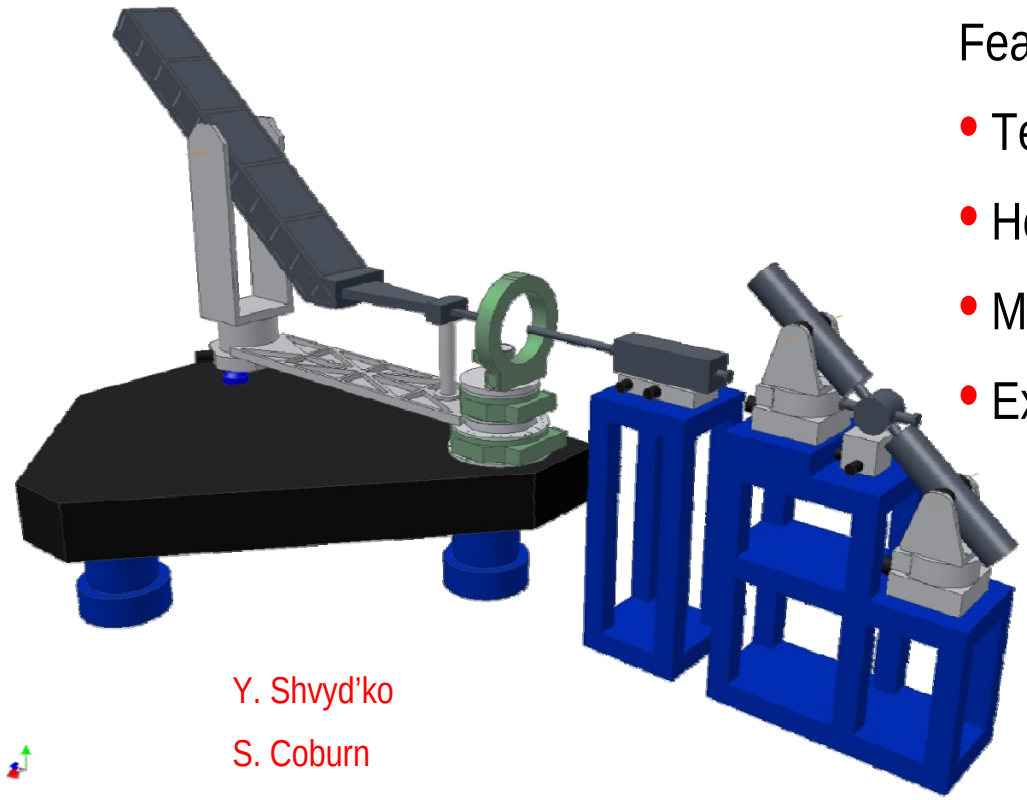
Schematics of 0.1-meV End Station

- Novel design featuring asymmetric backscattering optics (Yu. Shvyd'ko)
- Operate at 9.1 keV, near the peak of undulator spectrum



- Requires substantial R&D effort
- Limited acceptance for the analyzer

0.1 meV Spectrometer

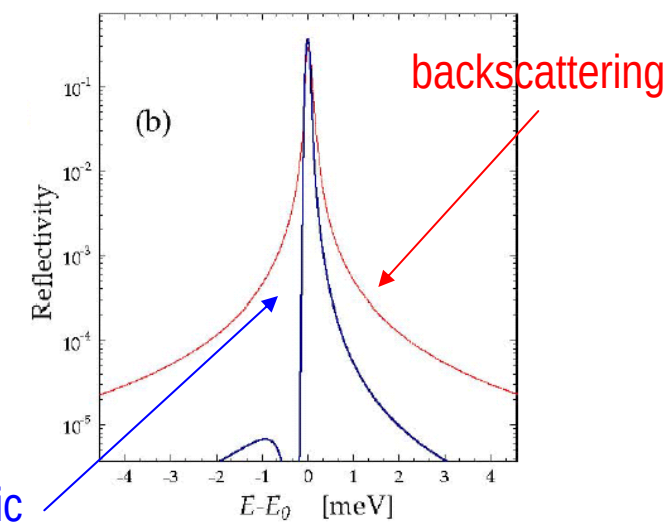


Y. Shvyd'ko

S. Coburn

Features

- Temperature scanning of energy transfer
- Horizontal diffraction plane
- Micron-sized spot.
- Extremely clean resolution function.

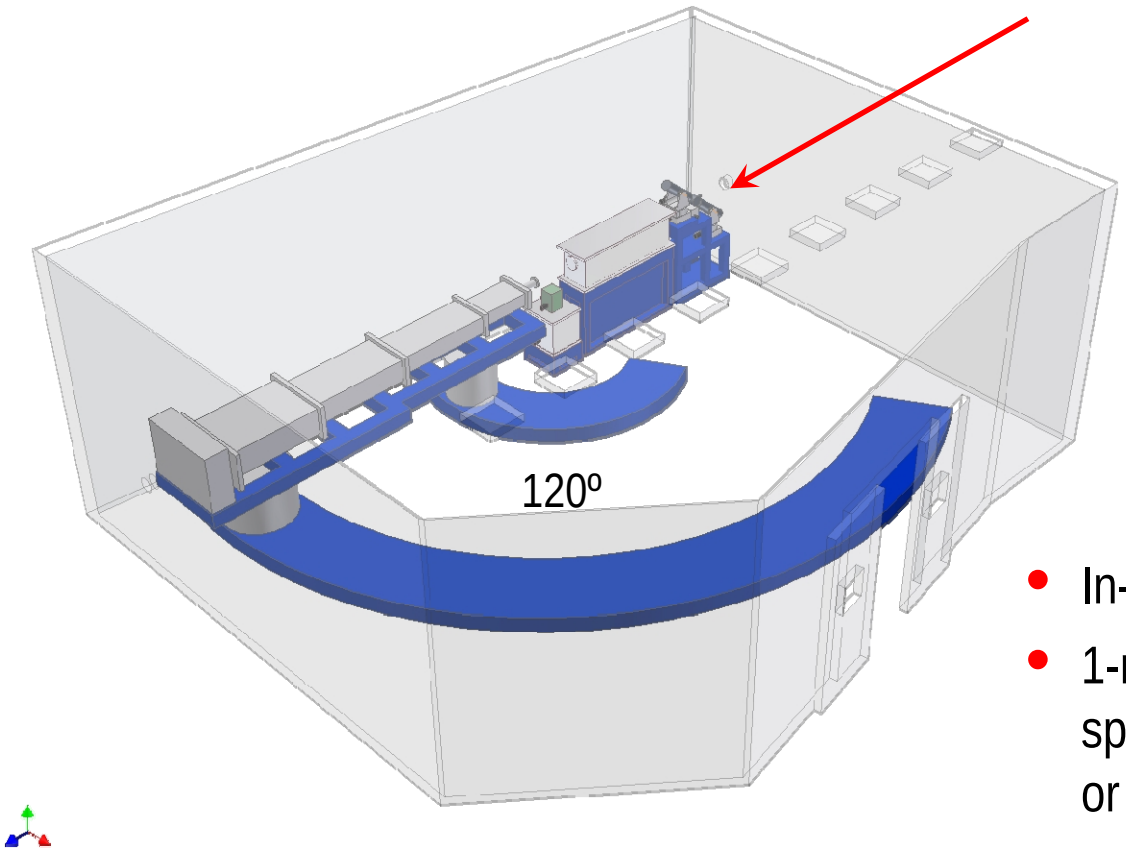


NSLS-II 3m U19	>1 x 10^9 phs^{-1} at 0.1 meV
APS 5m U30	1 x 10^9 phs^{-1} at 1 meV
Spring-8 4.5m U35	5 x 10^9 phs^{-1} at 1 meV

Schematics of 1-meV End Station

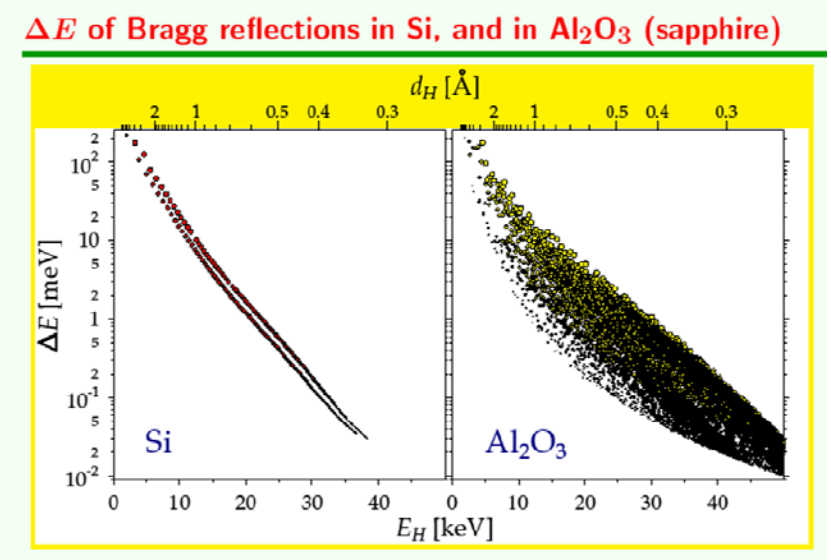
- OPTION 1: in-line HRM based on the CDDW scheme
  - require a collimating mirror
  - clean resolution function
  - part of the R&D process for achieving the 0.1-meV resolution
  - spectrometer could be a replicate of the 0.1-meV one optimized for 1-meV resolution, or
  - one that utilizes backscattering spherical analyzers made of sapphire or quartz crystals for large acceptance solid angles
- OPTION 2: backscattering HRM based on existing concept (but not with Si)
  - use sapphire or quartz crystals for 9.1 keV, quality of which is still a concern (more later)
  - large resolution function tail
  - require double Si(111) reflections to lift backscattered beam
  - compatible with spectrometer using spherical analyzers made of sapphire or quartz crystals
- Common to both options
  - Spectrometer arm to cover up to 120º scattering angle, requiring double ¼ wave plates

1-meV Spectrometer (Option 1)



- In-line CDDW HRM
- 1-meV end station with backscattering spherical analyzers made of sapphire or quartz crystal
- Large acceptance solid angle
- Poor sapphire and quartz crystal quality a concern

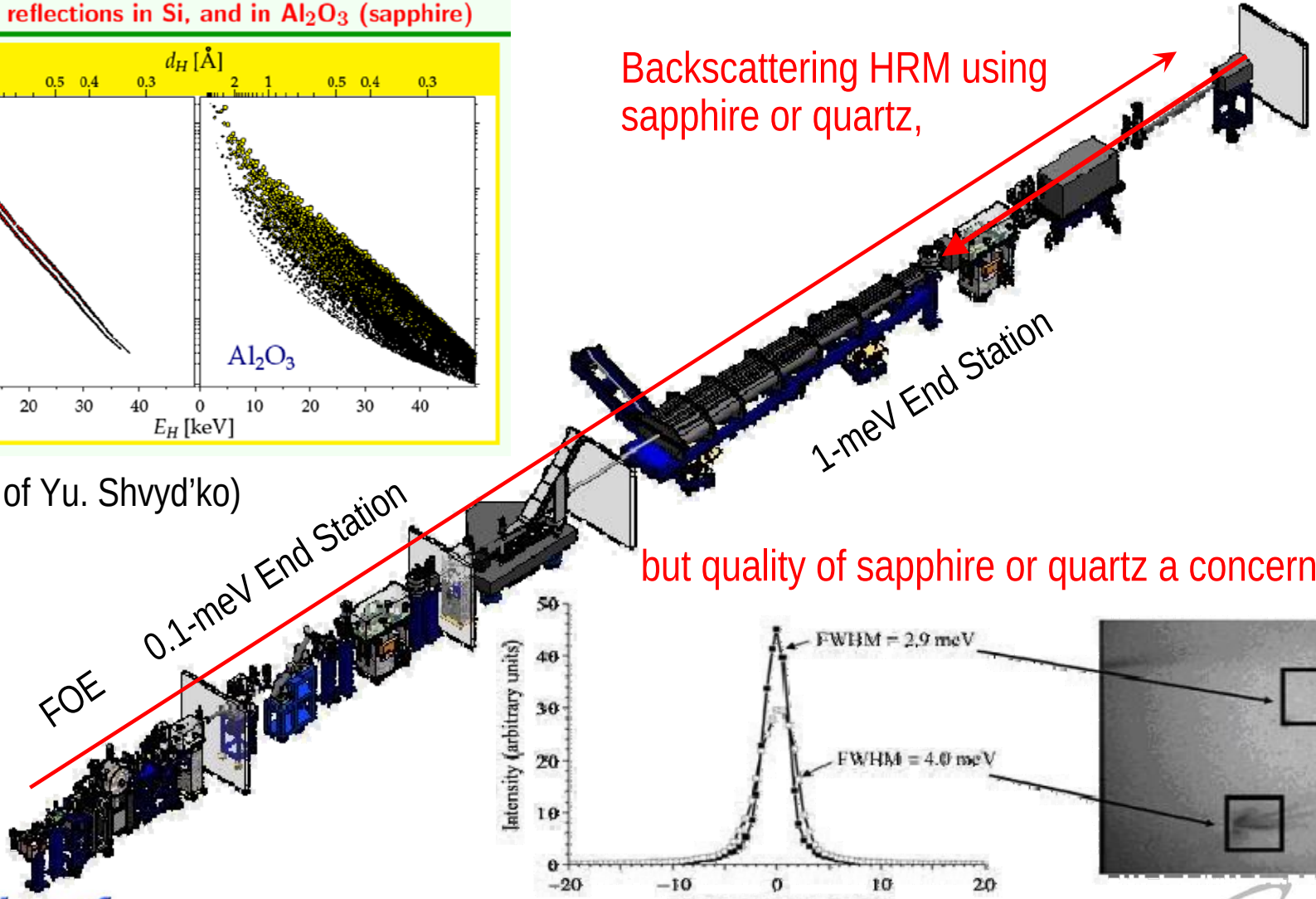
1-meV Spectrometer (Option 2)

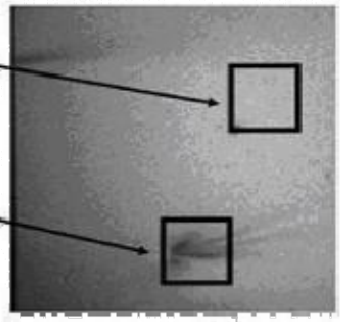


(Courtesy of Yu. Shvyd'ko)

Backscattering HRM using sapphire or quartz,

but quality of sapphire or quartz a concern





(Courtesy of A. Baron)

Outstanding Issues

- The type of straight section (low-β vs high-β) to be used (by end 2008, prelim. design)
  require careful evaluation involving ray tracing through optics on the ultimate flux and spot size delivered to the sample
- Multiple undulators on extended straight for more flux (depends on AS design)
  increase of heat load needs careful attention, so as the implications on the accelerator systems
- DCM: cryogenic cooled Si vs water cooled Diamond (by end 2010, final design)
  issues are vibration stability of cryogenic cooling vs water cooling, quality of diamond crystals, etc.
- CDDW scheme to achieve 0.1meV HRM: Substantial R&D effort required (by end 2011, final design; decision on the backscattering mono should be made before then)
- CDW scheme to achieve 0.1meV analyzers with 5-10mrad (H&V) angular acceptance: The biggest R&D and engineering challenge (by end 2011, final design)
- Risks with current approach and mitigation strategies to manage these risks:
  1meV would be possible, 0.1meV remains a real challenge, seek alternative schemes

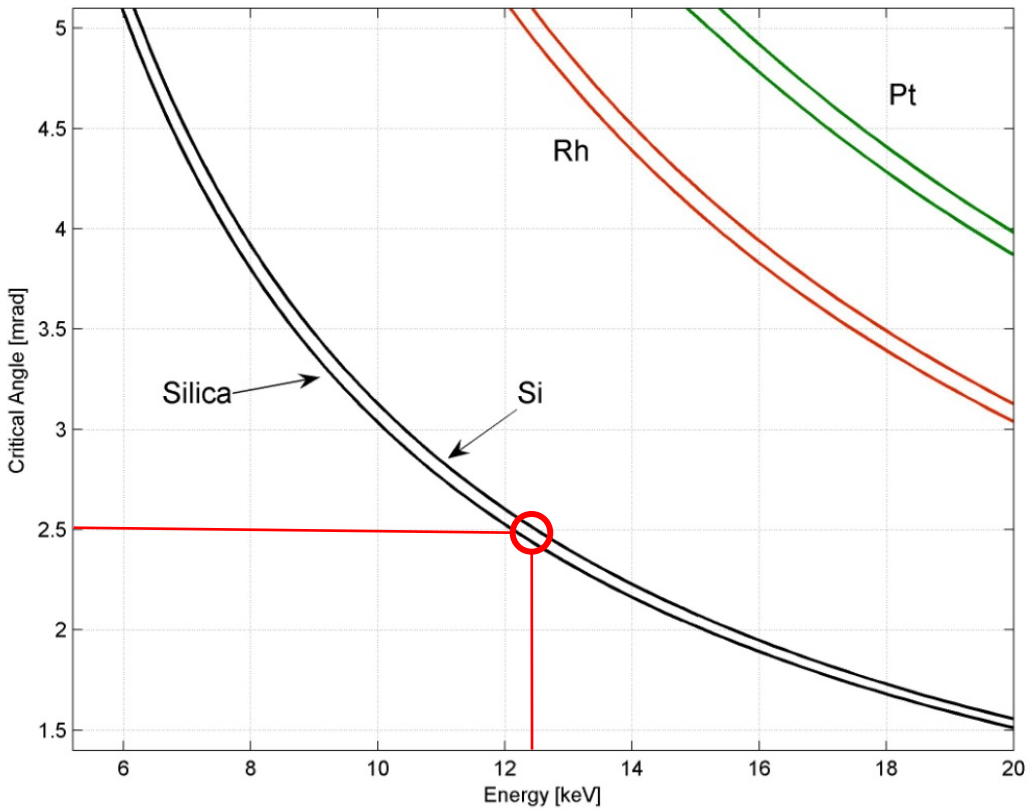
Cost Estimate

WBS	Item	Cost (k$)
1.04.05.01	Undulator Beamline 1 Inelastic X-ray Scattering	9,940
1.04.05.01.01	Enclosures	1,151
1.04.05.01.02	Beam Transport	685
1.04.05.01.03	Utilities	336
1.04.05.01.04	White Beam Components	0
1.04.05.01.05	High Heatload Optics	977
1.04.05.01.06	Beam Conditioning Optics	1,921
1.04.05.01.07	Personnel Safety System	183
1.04.05.01.08	Equipment Protection System	86
1.04.05.01.09	End Station 1	2,522
1.04.05.01.10	End Station 2	0
1.04.05.01.11	Beamline Controls	674
1.04.05.01.12	Beamline Control Station	36
1.04.05.01.13	Beamline Management	1,369

Summary

- These IXS instruments to be built at NSLS-II would feature unprecedented performance with up to 0.1-meV resolution and flux of over $1x10^9$ photons/sec/0.1meV at ~ 10 keV, taking full advantages of the NSLS-II's superior performance at this energy.
- There are critical decisions to be made on undulator(s), type of straight section, and high heatload components, but those are believed to be manageable within the timeline of the project.
- There are technical challenges, particularly concerning the way to achieve the 0.1-meV resolution, that require active R&D. The spectrometer design, and to some extent the beamline design, will depend on the outcome of the R&D program.

Reflectivity of Mirrors



Incident angle versus cut-off energy

Parameters of Mirrors

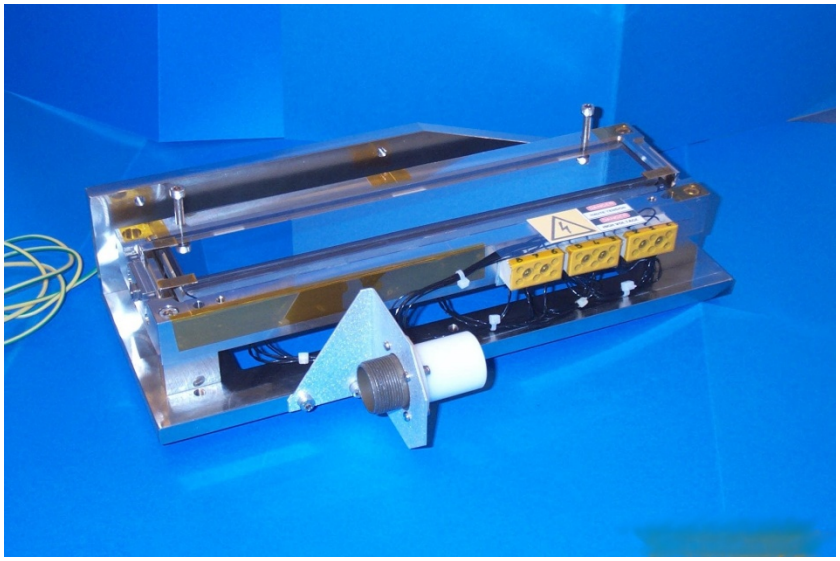
- Parameters for low- β , high emittance (0.55 nm-rad), and 4σ (H) x 4σ (V) opening
- For high- β straight, horizontal mirror length can be shorter thanks to the smaller beam size

Mirror	Optical distance from source, m	Incl-dence angle, mrad	Coating	Beam Footprint, mm		Bent radius, m	P, m	Q, m
				Horizontal	Vertical			
VCM	31.88	2.5	Silica	3.2	291	25220	31.88	∞
VFM	39.15	2.5	Silica	3.8	291	336	- ∞	0.42
VCM'	40.33	5	Rh	7.6	1014	338	0.76	∞
VFM	74.46	2.5	Silica	3.8	291	516	- ∞	0.645
HFM	38.05	4.5	Rh	848	0.9	650	38.05	1.52
HCM	38.05	4.5	Rh	846	0.9	16911	38.05	∞
HFM	73.38	4.5	Rh	848	0.9	776	- ∞	1.745

Notes: 1) Footprint of the beam at VCM corresponds to angular acceptance of 10 mrad (H) and 5 mrad (V). To increase angular acceptance the VCM has Rh coating and higher angle of incidence.

Collimating and Focusing Optics

- Candidate: Bimorph mirrors



- Supplied by SESO
- Multiples of 150mm in length
- Each segment can be bent independently (2 electrodes for cylindrical and 4 electrodes for elliptical)
- Bimorph can in principle correct its own tangential polishing slope errors and also correct for tangential errors introduced by other optics
- KB bimorph pair can in principle correct for sagittal and tangential errors