Thoughts on HEX Optics

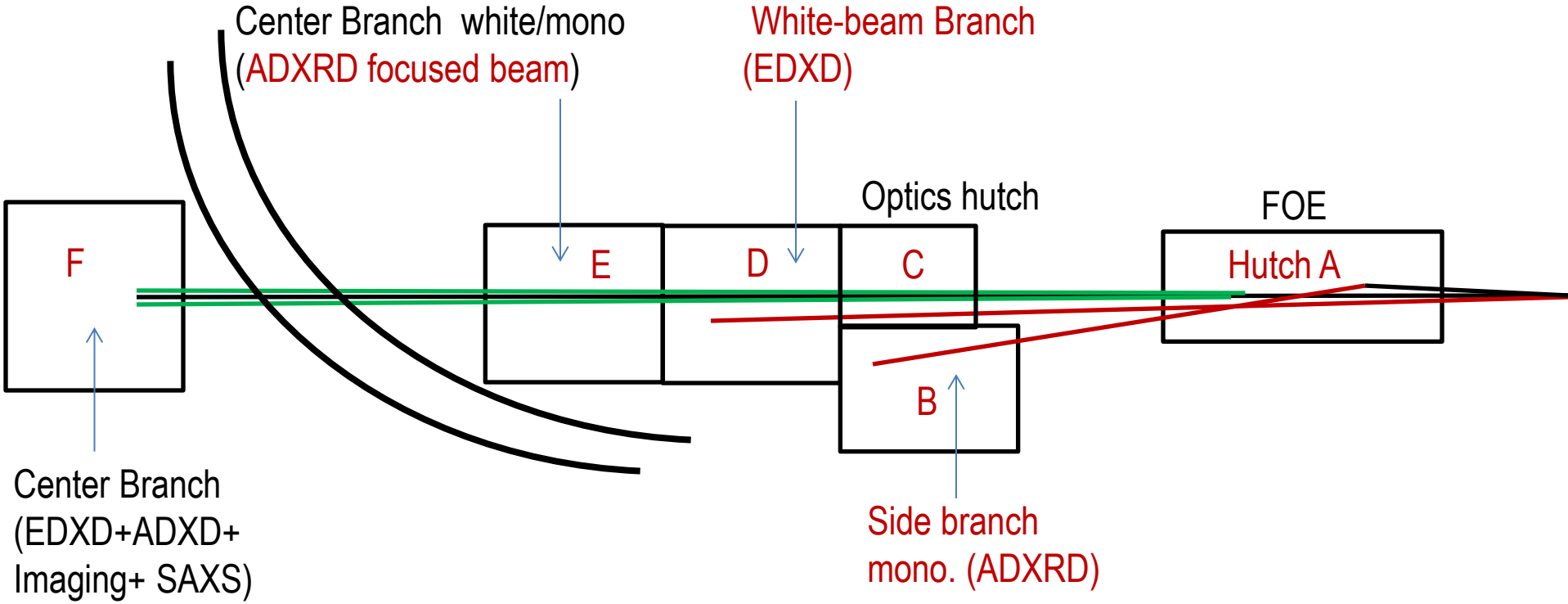
HEX PDR Meeting 4/26/2018

Zhong Zhong
Beamline Scientist

Outline

- Beamline Optical design
  - Optical scheme
  - Imaging Monochromator Design and Specifications
  - Micro-focusing Optics Design and Specifications
  - Heat load considerations
- Summary notes

HEX Beamline Layout

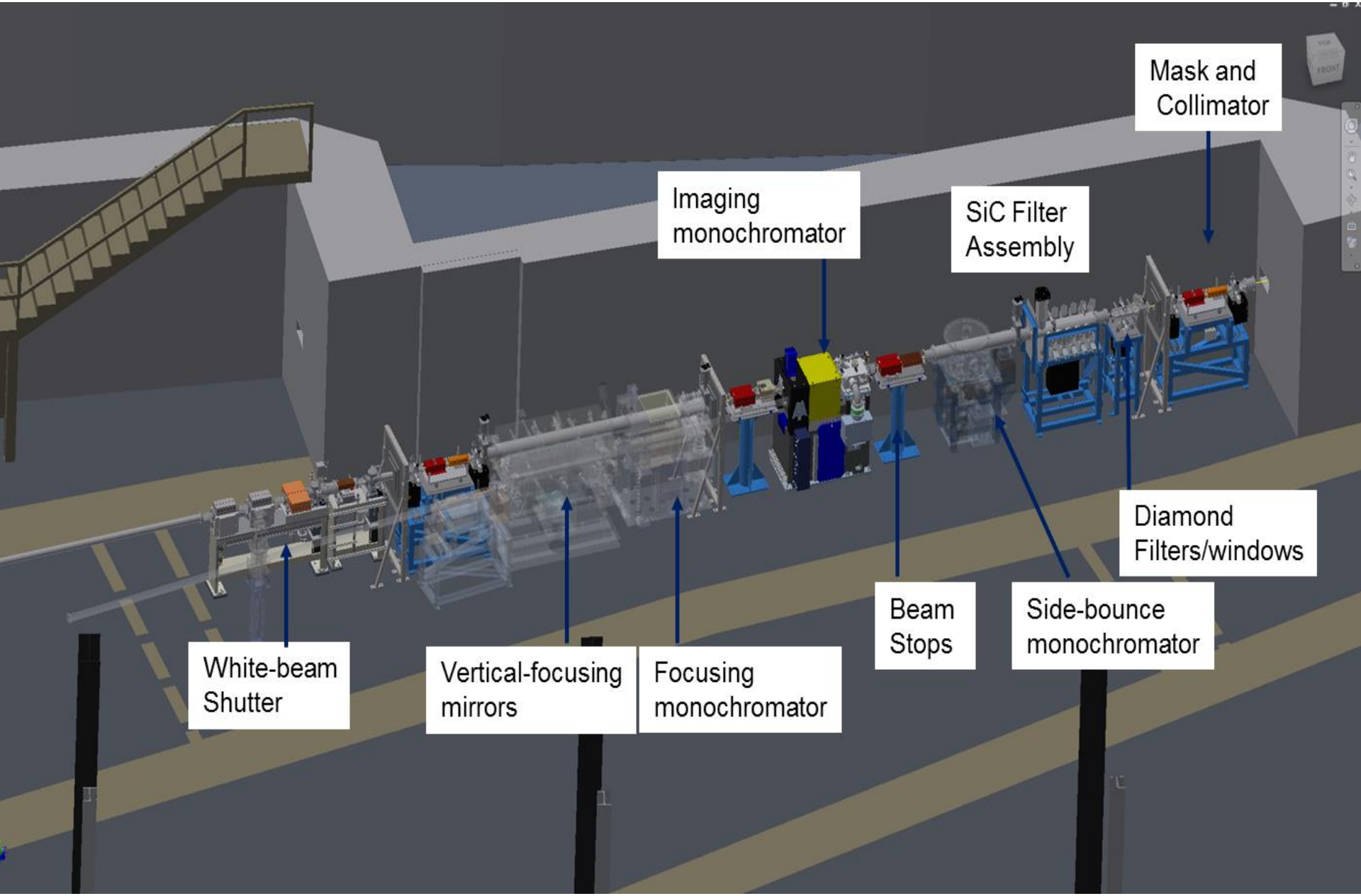


Center branch optics and endstation F is in the scope

Optics and endstations for white beam (D) and side (B) branches are not in current scope

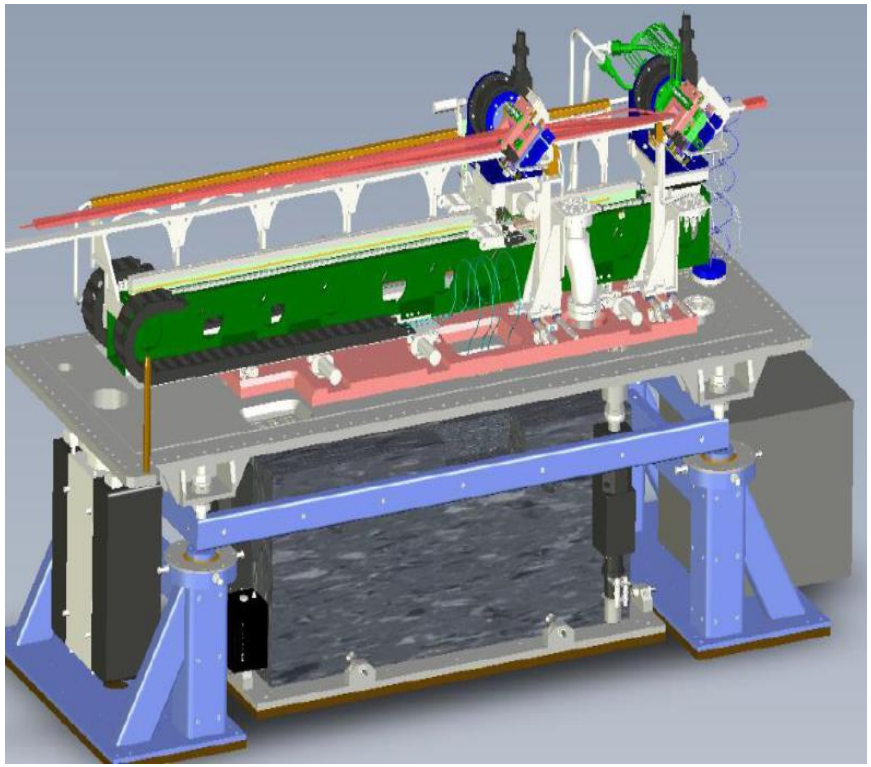
B and D hutches may be de-scoped if needed

HEX Optical Layout



Optics

	Side branch	Center Branch	White-beam Branch
Monochromator	One-bounce bent-Laue	Sagittal focusing mono Imaging mono	N/A
Mirror	Vertical-focusing	Vertical-focusing	N/A
Mode	Monochromatic	White/Monochromatic	White

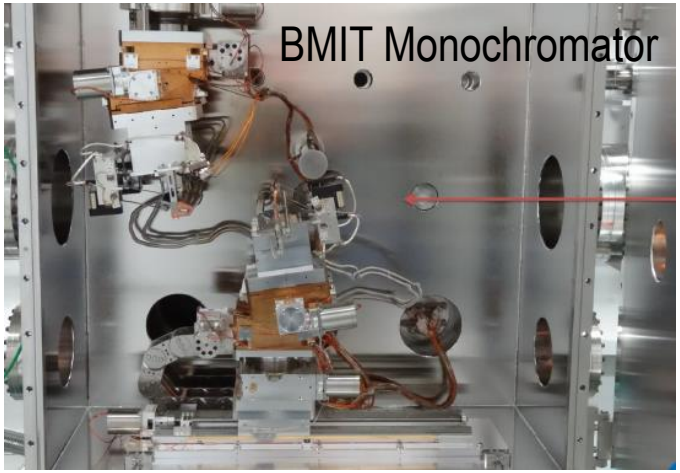


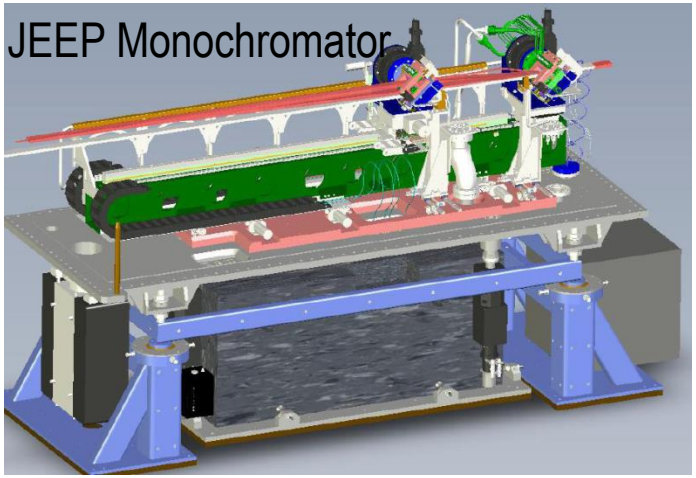
Imaging monochromator

- Meridionally bent asymmetric crystals
- Use small offset – 25 mm – compact and stable
- Proven design used at NSLS, JEEP, Australian Light Source and BMIT

Imaging Monochromator

- High-energy x-rays are especially suitable for imaging batteries, engineering materials and earth science samples
- Simulations show that it can be implemented at the HEX to provide the high-energy x-rays at a flux of 10^{11} ph/s/mm^2 at sample
- Removable from the white beam. It will allow EDXRD (high spatial resolution and depth resolution, low angular resolution) and imaging on the same sample, greatly enhancing the HEX scientific programs.
- When the monochromatic beam size is reduced by slits, it can be used for ADXRD.





Design Ideas and Parameters

- HEX center branch is white-beam compatible. Thus a small offset of 25 mm is chosen to minimize distance between the two crystals – compact design and higher stability

- Monochromator first crystal and beam stop must be removable/EPS interlocked to allow white-beam operation.

- Source to monochromator distance (f1): 31 m

- Monochromator to sample distance (f2): 73 m

- Large (100 mm x 20 mm) field of view at the F station in the satellite building.

- Adjustable x-ray energy 30-150 keV

  - Energy change without readjusting bending

  - Energy resolution is not important for imaging. However, if possible, the monochromator should offer a high-resolution mode for possibly using it for diffraction in the future ~ 10^{-3} dE/E

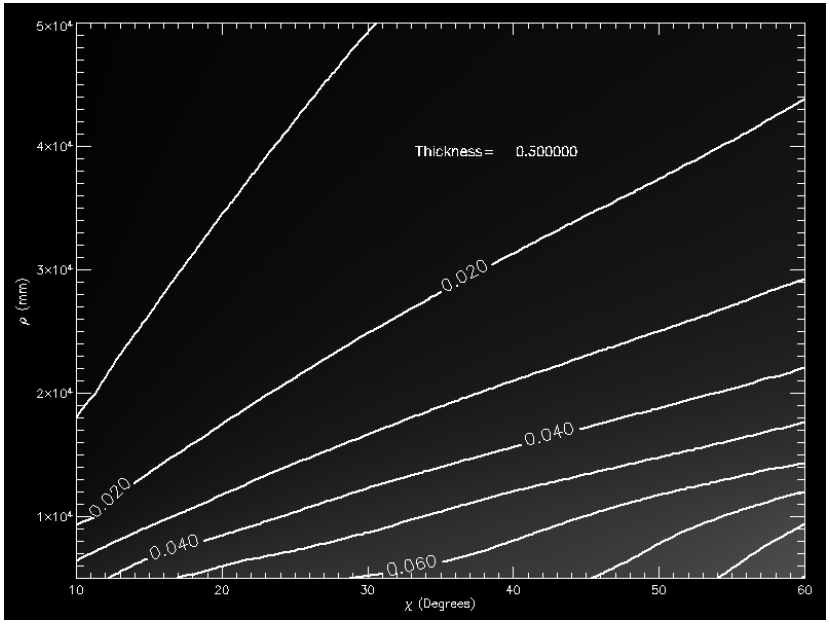
Monochromator Design

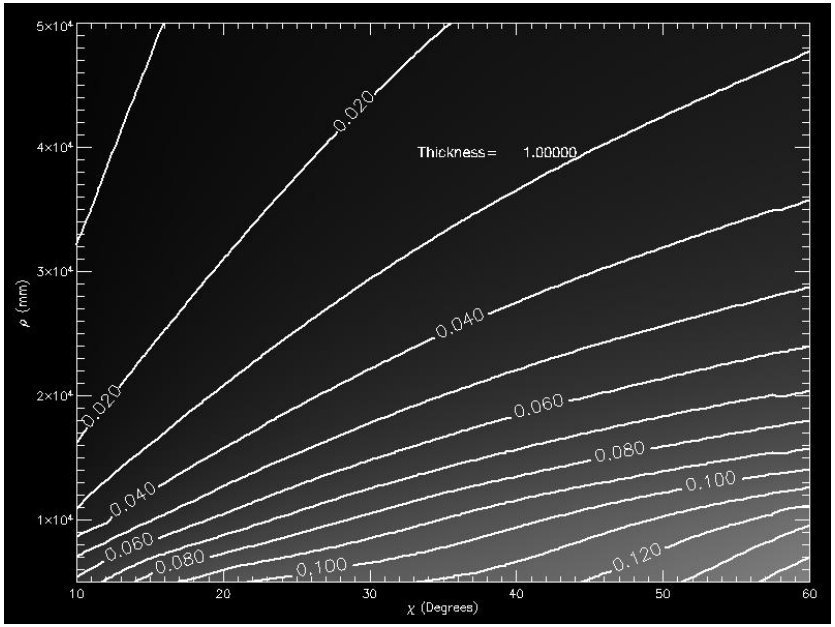
- 4 mm thick SiC filter to control heat load on monochromator
- Both crystals are meridionally bent towards the source to minimize energy difference between –top and –bottom parts of the beam
- Inverse Cauchois geometry, at ~40 m bending radius gives zero energy difference. However, 10-20 m bending radius yields acceptable energy-difference, and larger band-width and higher intensity
- Asymmetric crystals to enhance bandwidth
- 1-3 mm thick crystals
- Consider the second crystal having slightly larger bending thickness than first crystal to achieve flat-top rocking curve – BNL MECT design used at NSLS X17
- Will use water-cooling to reduce cost and simplify operations

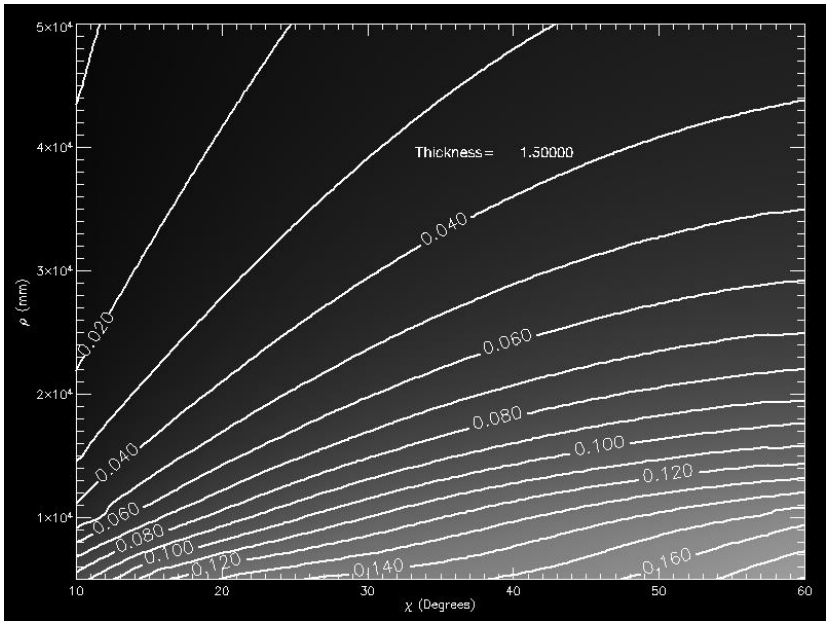
Considerations for optimization

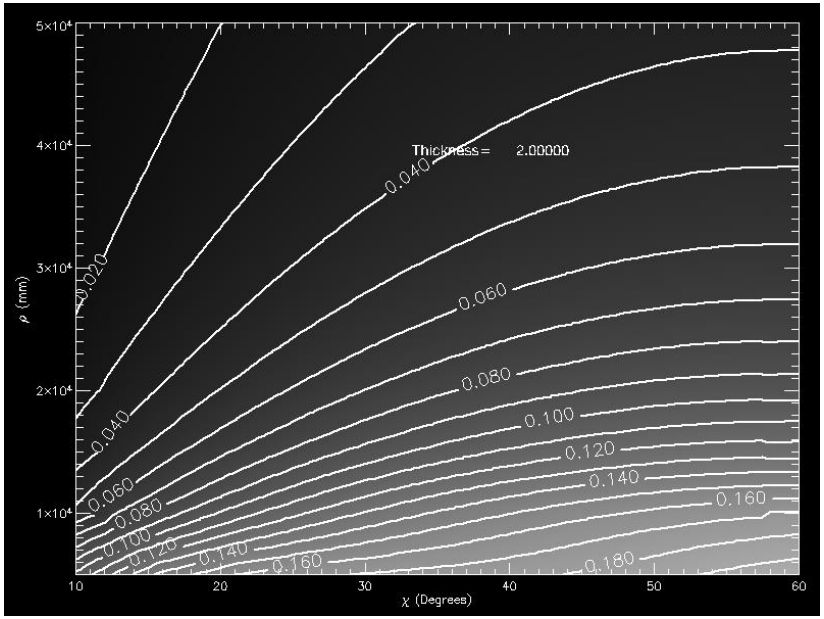
- Large parameter space: Asymmetry angle, crystal thickness, bending radius
- Asymmetry angle: larger = larger bandwidth = higher flux, if two large, the beam foot-print on crystal increases
- Thickness: Thicker crystal = lower flux for low energy, would like to be able to image at 30 keV
- Bending radius: 40 -50 m gives best energy resolution, 10-20 m gives higher flux
- An IDL program was written, using lamella model for bent-crystals, to explore the parameter space.

Optimization 111, 50 keV









Analysis of Optimization Results

- Benefit of asymmetry angle “levels off” after about 40 degrees. Thus the “symmetrical crystal cut” of 35.3 degrees asymmetry angle, with crystal surface being 100, is appropriate

- Smaller bending radius results in higher flux, at the cost of energy-difference between –top and –bottom of beam. The flux benefit “levels off” at smaller than 10 m radius.

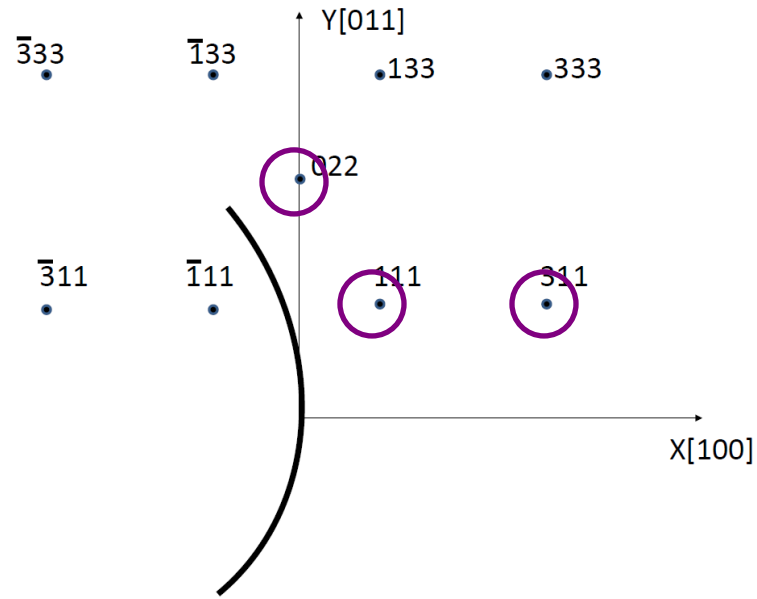
- 1.5- 2 mm allows reasonable 30 keV performance. Thicker crystals benefit higher energies. – Choose 2 mm for baseline design

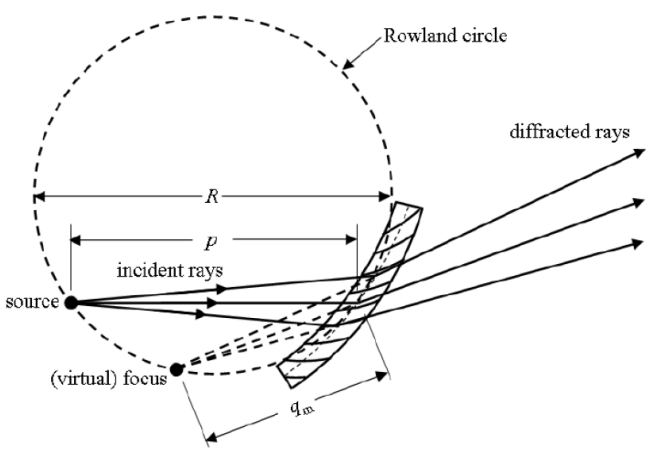
- Conclusion: 35.3 degrees chi, 1.8 mm (1st crystal) & 2.2 mm (second crystal) thickness, 10-50 m bending radius, 25 mm gap, +- 35 deg. angle range (if possible)

Survey of similar monochromators world-wide

	BMIT (CLS)	JEEP (Diamond)	UHX (ShangHai)	IMBL (Australia)	CAMD	HEX (NSLSII)
Asymmetry angle (degrees)	15	44	45	15	35.3	**35.3**
Reflection	111 & 220 (either/or)	111	111	111, 311 via rotation	111	**111, 220 & 311 via rotation**
Thickness (mm)	2.0	4.0	4.0	1.0	0.7	**1.8 1st crystal 2.2 2nd crystal**
Offset (mm)		50	50	20	8-25	**25**
Energy range (keV)	25-150	53-150	45-150	30-100	30-80	**30 – 150**
Cooling	Water, In-Ga trough	Cryogenic	Cryogenic	Water, In-Ga bath	Water, one-side	**Water, one-side**
Bender	2 Leaf Springs	2 Leaf Springs	2 Leaf Springs	2 Leaf Springs	2 Leaf Springs	**2 Leaf Springs**

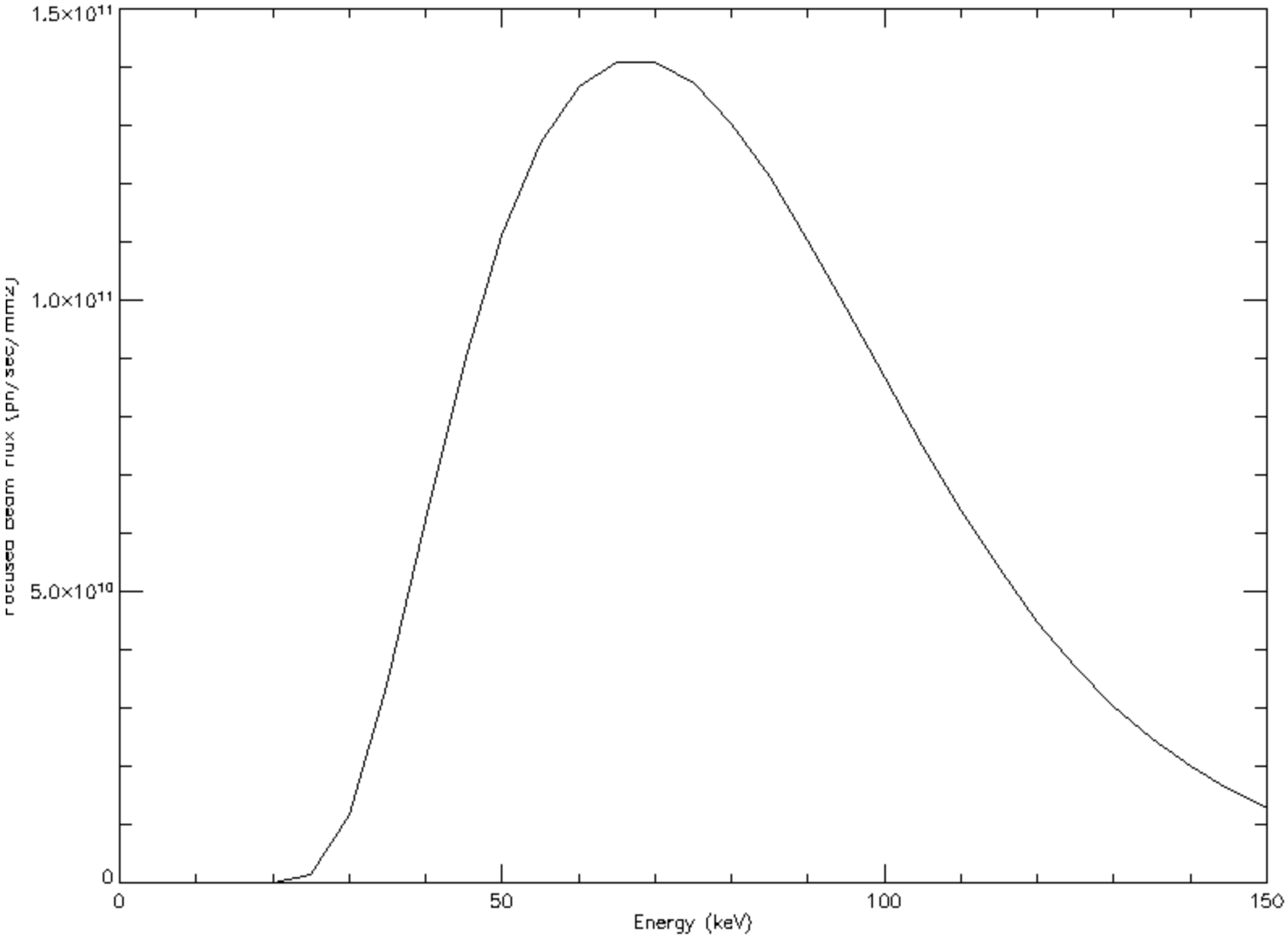
100 xtal, choice of 3 reflections 111, 022 & 311



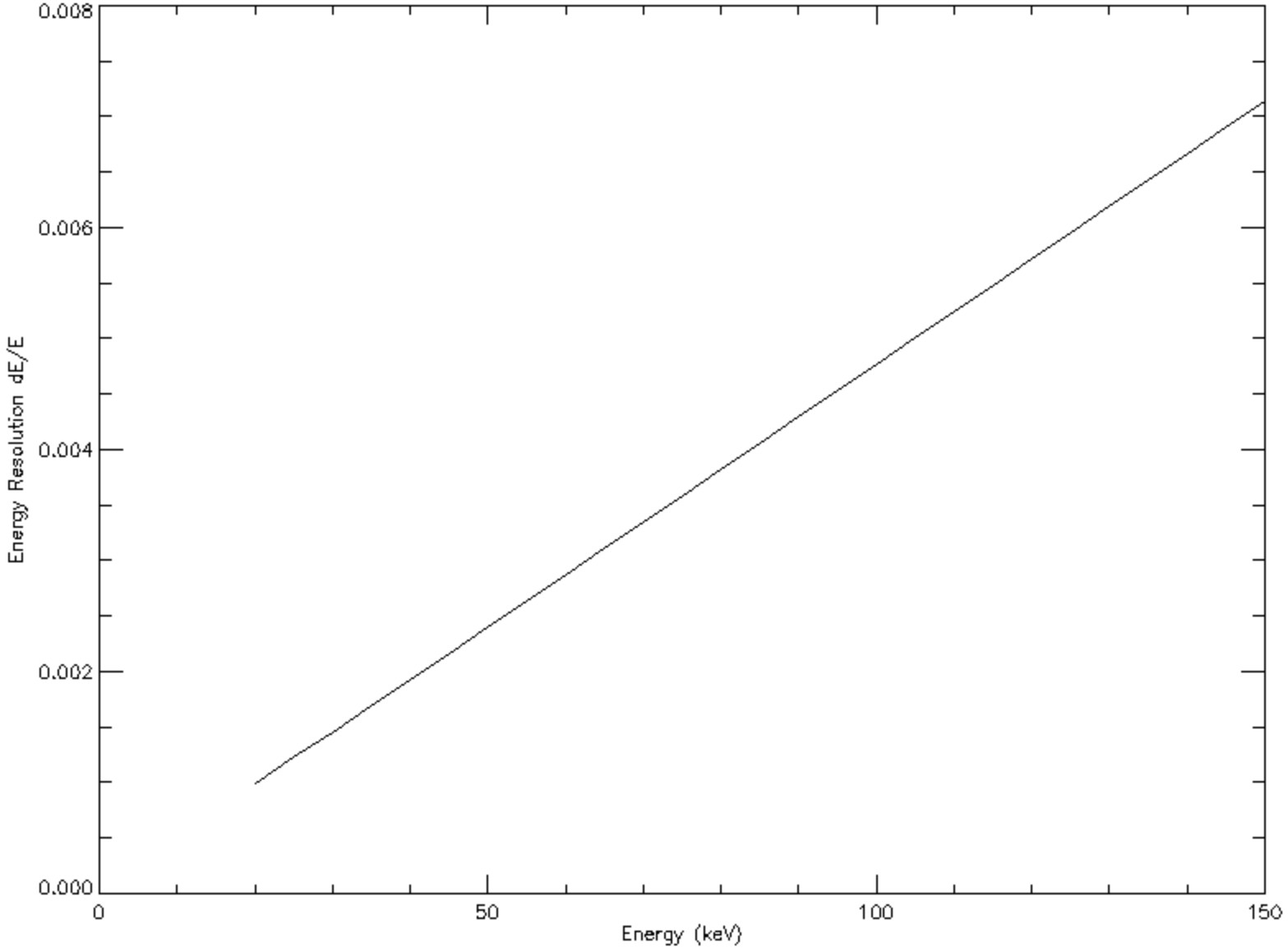


- Symmetrical crystal design, minimizes confusion
- 111 has large (35.3 degrees) asymmetry angle, high flux for imaging
- 022 is symmetrical reflection, high resolution, low flux, has second harmonics, for diffraction
- 311 is has high resolution and moderate flux, no second harmonics, candidate for diffraction
- 022 and 311, both about 30 degrees from nominal 111 position.

111 Reflection, T=2 mm, rho=30 m



111 Reflection, T=2 mm, rho=30 m

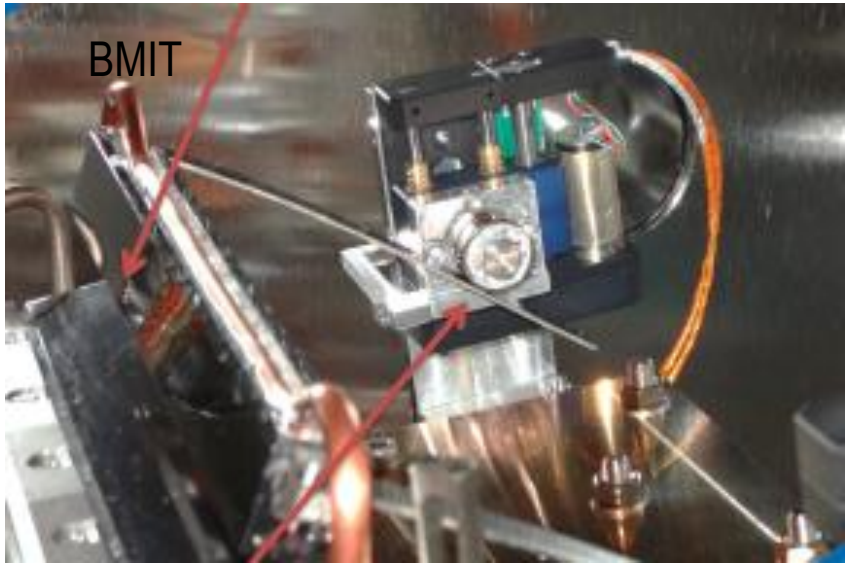


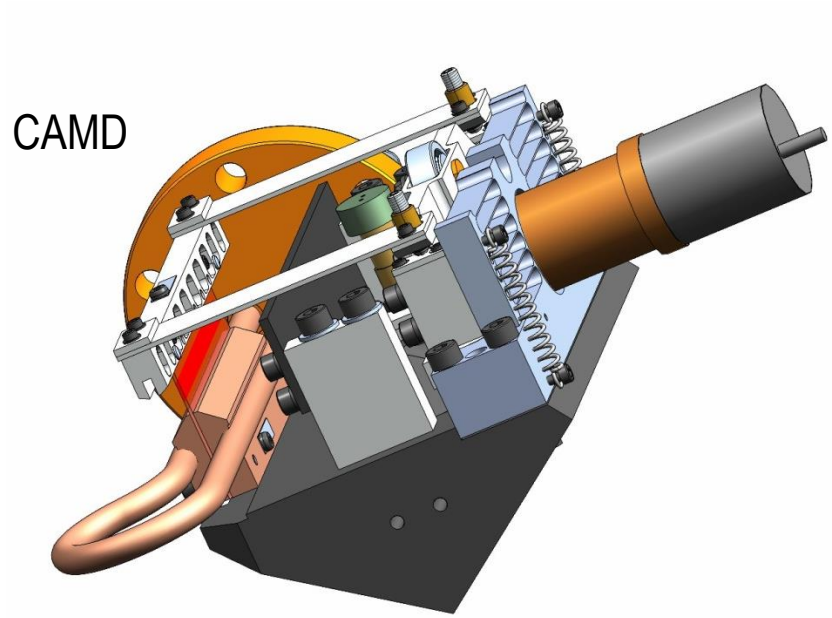
Simulation for 111 reflection, T=2 mm, Rho=20 m

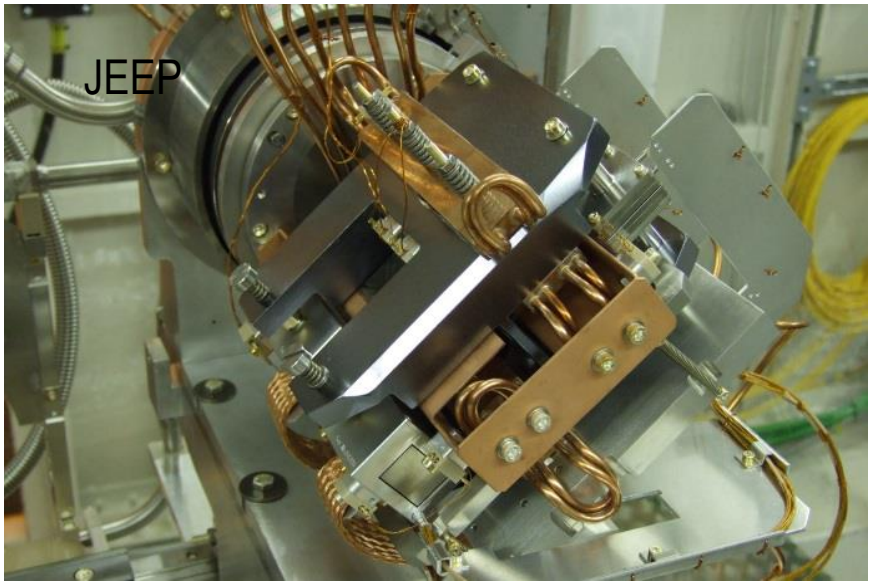
Energy(keV)	30	40	50	60	70	80	90	100
Bragg angle (deg)	3.779	2.833	2.266	1.888	1.618	1.416	1.259	1.133
Shift (mm)	188	252	315	379	442	505	568	631
dE/E ($x10^{-3}$)	1.4	1.9	2.4	2.8	3.3	3.8	4.2	4.7
Integrated Reflectivity (micro-radians)	35	53	62	67	69	70	70	66
Reflectivity (%)	0.44	0.67	0.78	0.83	0.86	0.89	0.85	0.82
Flux in F hutch (10^{11}ph/s/mm^2)	0.12	0.62	1.1	1.4	1.4	1.3	1.1	0.86

- At 150 keV, 1 m between crystals, the flux is still reasonable at $2x10^{10}$ph/s/mm^2.

Bending Mechanism







Specification for Imaging Monochromator

Component	Specification	Notes
First Crystal	12 mm (V) by 40 mm (H), 1.8 mm thick +- 35 deg. rotation in plane, 0.001 deg. resolution Bending radius (towards source) 10 m – infinity 2 leaf spring bender	Water-cooling required
Second crystal	12 mm (V) by 40 mm (H), 2.2 mm thick +- 35 deg. rotation in plane, 0.001 deg. resolution Bending radius (towards source) 10 m – infinity +- 35 deg. rotation in plane, 0.0001 deg. resolution +- 2 deg. tilt, 0.001 deg. resolution 2 leaf spring bender Distance to first crystal: 150 mm – 1 m z translation along beam 25 mm Y offset from first crystal	Water-cooling not required
Compton scatter shield	Water-cooled copper shielding around first crystal	
Beam stop	Water cooled copper block, normal incidence OK, coated with phosphor	
Vacuum vessel and support	0.6 m width x 1.5 m length 0-100 mm vertical adjustment to switch between monochromatic beam and white beam, 1 micron resolution position sensor required for EPS 2 Quartz view ports of 6 inch diameter	
Diagnostic flag	Near the exit port of vacuum vessel, 50 mm x 50 mm area to capture both transmitted and diffracted beams from 2nd crystal, 100 mm vertical motion	

Micro-focusing optics

The requirements for micro-focusing:

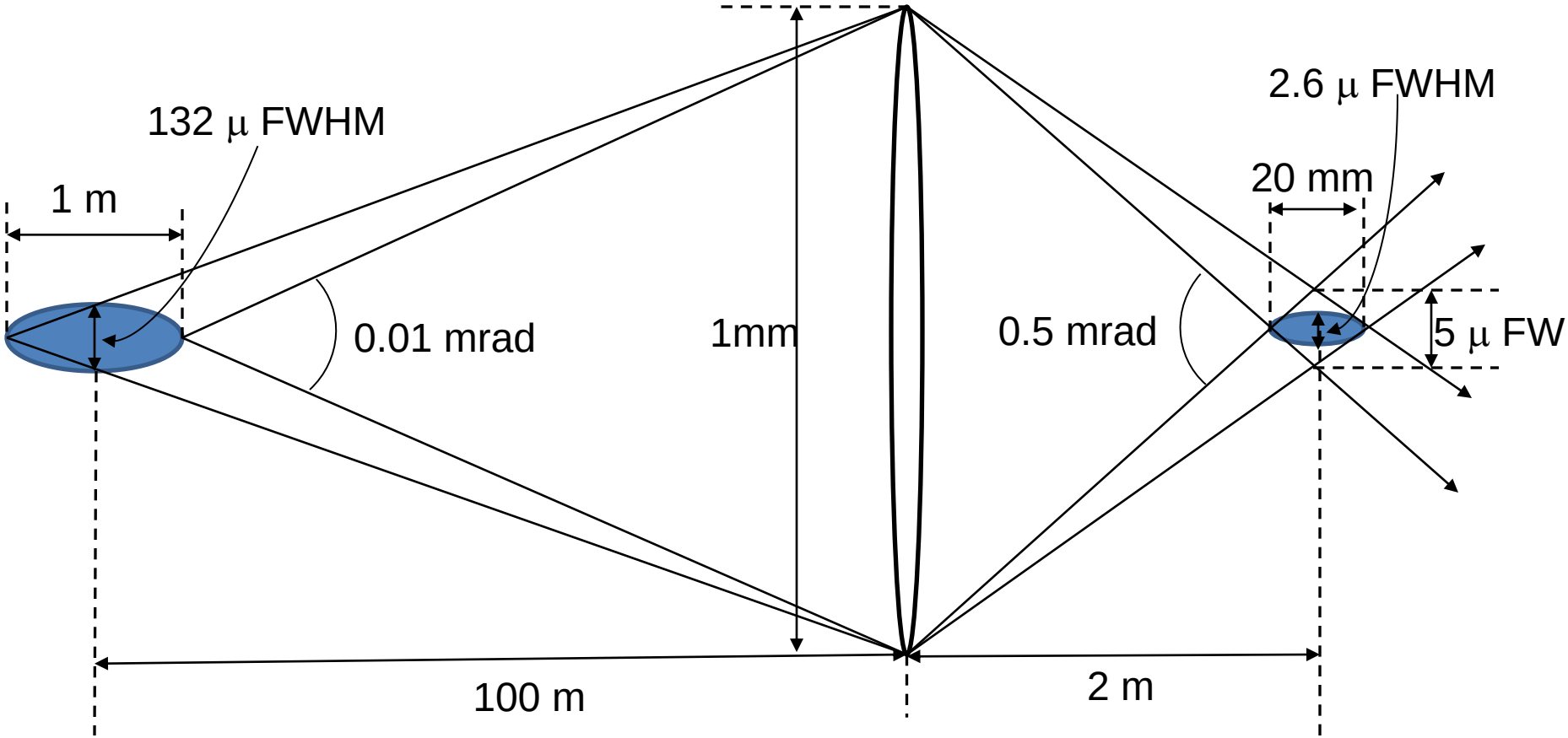
- Spot size of less than 10 microns
- Option for line focusing is desirable
- Focal distance of about 2 m. The source distance is 100 m
- Ease of alignment/operation preferred

	Aperture	Focal spot(μ)	Line-focus	Energy tunability	Price	In-line
K-B mirror	0.5 mm x 10 mm*	1	Yes	Easy	$400k	No
Bent Saw-tooth	1 mm x 10 mm	1	Yes	Relatively easy	$100k, R&D	Yes
Kinoform	0.3 mm x 0.1 mm	0.2	No	Difficult	$100k, R&D	Yes
CRL	~0.5 mm	1	No	Relatively difficult	$100k	Yes

* Assuming 0.5 m long mirror at 1 mrad incidence angle

- Consider the K-B mirror as the first option due to its commercial availability, good energy-tunability, Line-focus capability, and large aperture
- Bent Saw-tooth optics as second option due to low price, positive experience at APS-1ID, line-focus capability and large aperture.

Effect of source length on micro-focusing

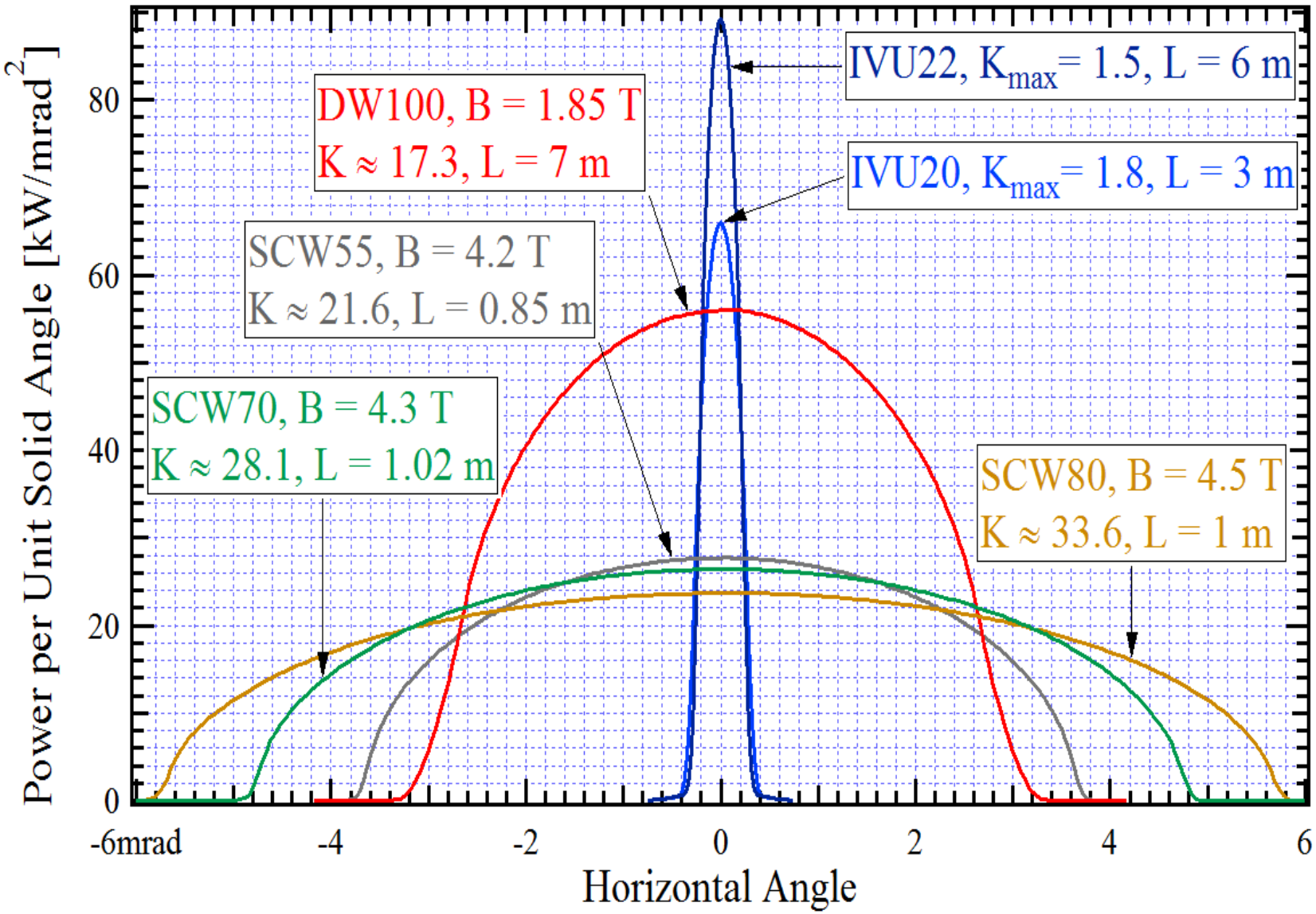


- The 1 m length of the wiggler at aperture of 0.01 mrad contributes to FWHM of 2.5 μ.
- Convolution of this with the 50X de-magnified source of 2.6 μ (H) x 0.14 μ (V) FWHM results in focal spot of 3.6 μ (H) x 2.5 μ (V) FWHM.
- Specify the figure errors of the focusing optics to contribute to <2μ in focal spot size.
- Slope-error <1 micro-radians at working distance of 2 m.

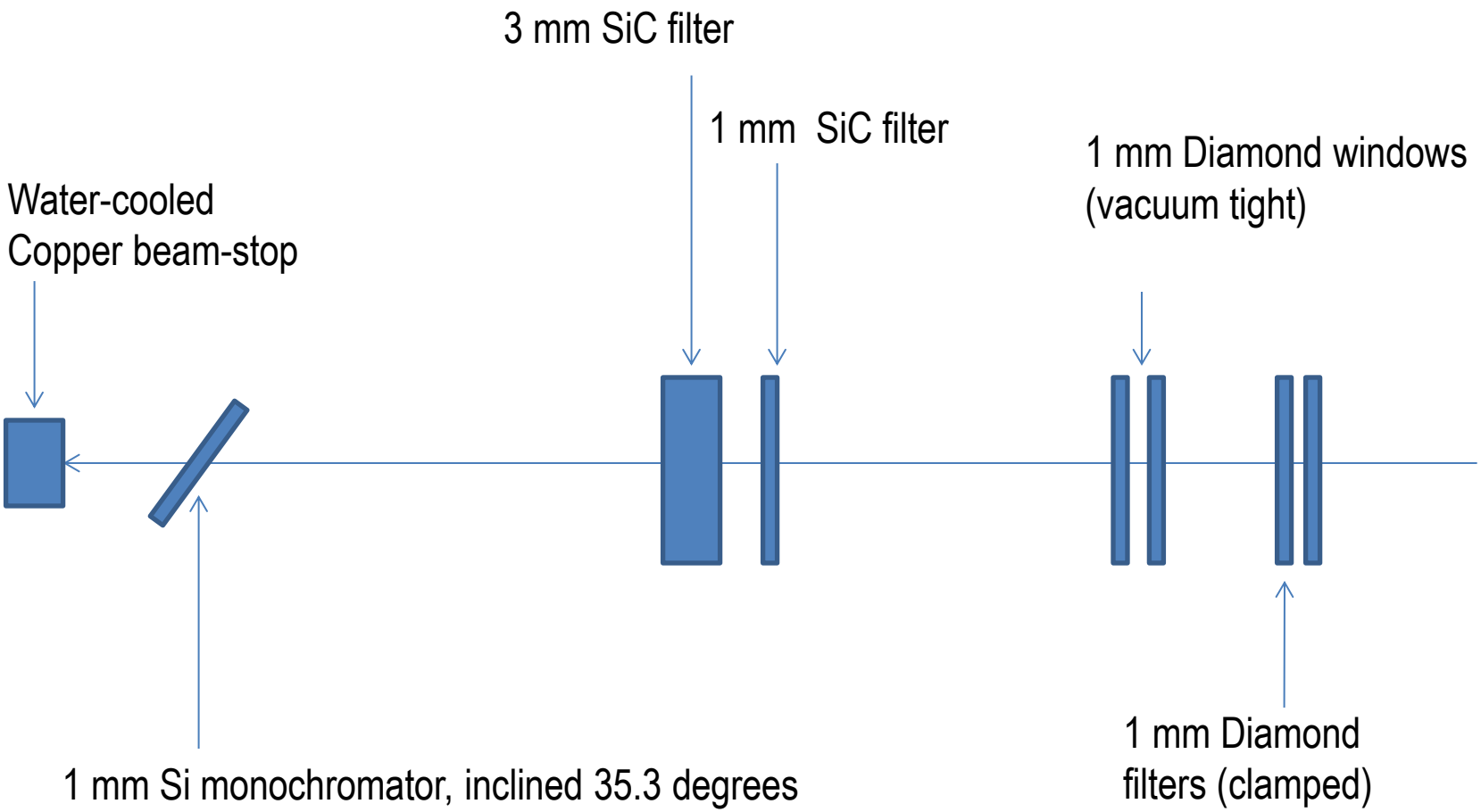
Specification for Micro-focusing Optics

Component	Specification	Notes
Micro-focusing optics	K-B mirrors (0.5 m length for each mirror) 30-~100 keV, 2m focal length, 1 micro-radians slope error Removable from the beam N2 or vacuum compatible	Desirable to have horizontal line focus

Heat load: manageable

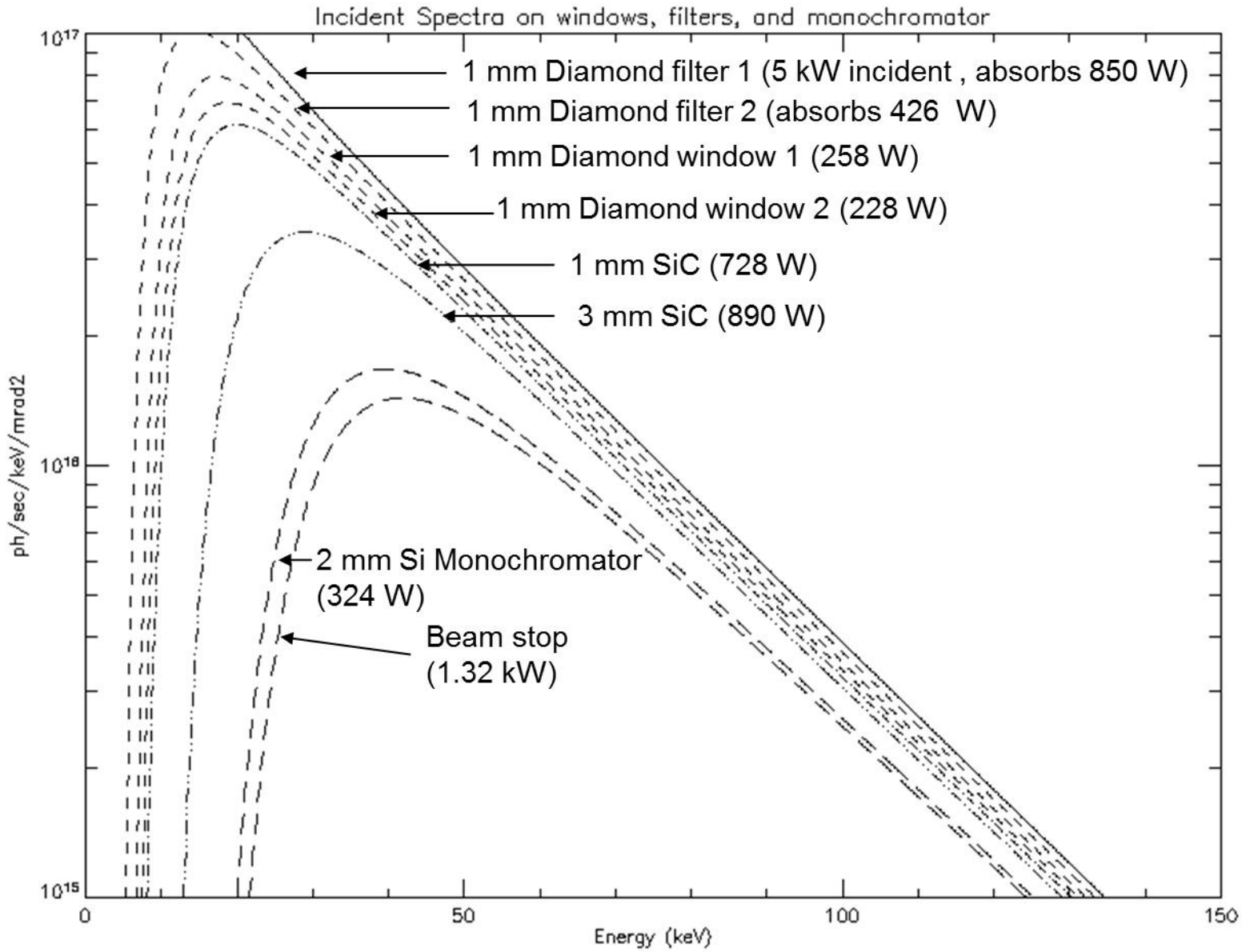


Model



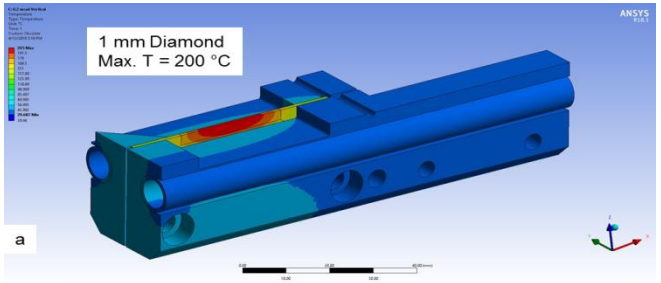
- Aim to make beamline passively safe without additional filter

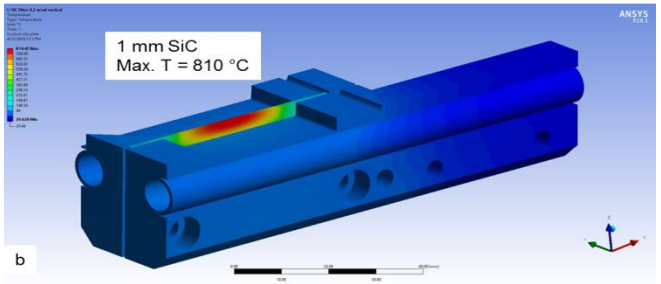
Absorbed Power



Heat load

	Material	Thickness Along Beam (mm)	Incident Power Density (kW/mrad^2)	Absorbed Power Density (kW/mrad^2)	Maximum Absorbed Power (W)
Diamond filter 1 *	Diamond	1	25.1	4.25	850
Diamond filter 2	Diamond	1	20.9	2.13	426
Diamond window 1	Diamond	1	18.8	1.29	258
Diamond window 2	Diamond	1	17.5	1.14	228
SiC filter 1 *	SiC	1	16.3	3.64	728
SiC filter 2	SiC	3	12.7	4.45	890
Monochromator *	Si	2	8.25	1.62	324
Beam stop	Cu	n/a	6.63	6.63	1326



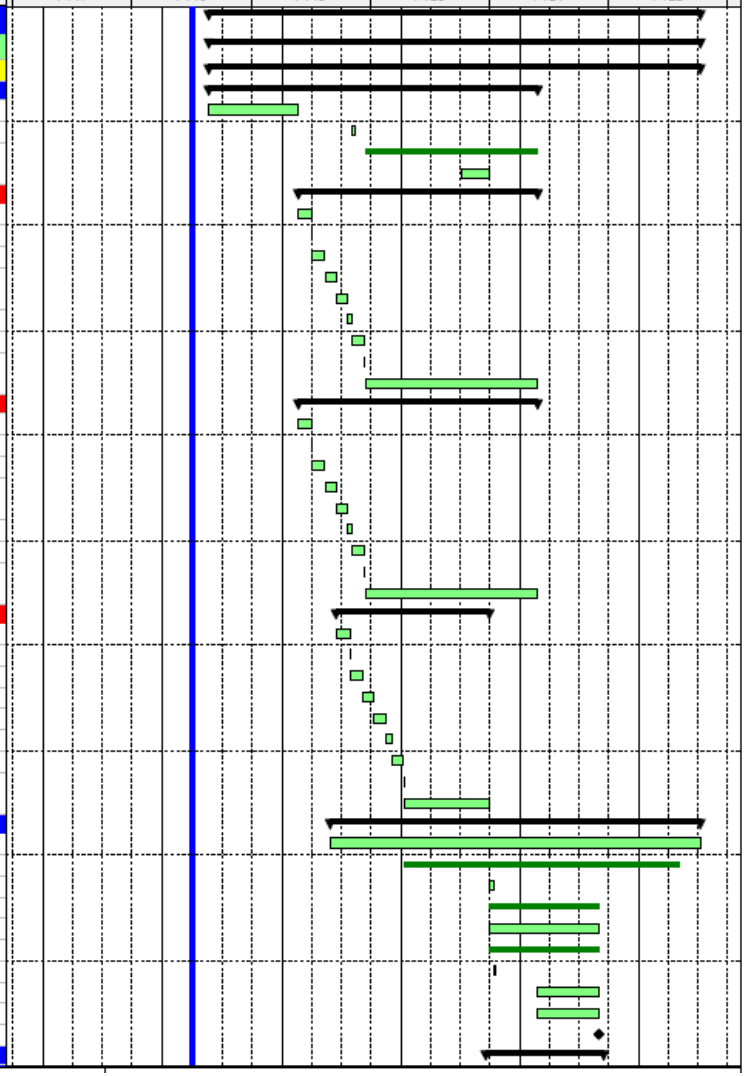


: Results of the power simulation. FEA are performed for components denoted by * to assure survivability.

Cost/schedule

HEX Partner Beamline — Estimation Layout — 17-Apr-18 09:13

Activity ID	Activity Name	Original Duration	Start	Finish	Budgeted Labor Units	Budgeted Nonlabor Units	Budgeted Total Cost	BNL_Fund
HEX Partner Beamline		**1033**	**22-May-18**	**08-Jul-22**	**13546**	**5119821**	**$7,333,429**	
HEX Beamline		1033	22-May-18	08-Jul-22	13546	5119821	$7,333,429	
HEX Beamline Construction		1033	22-May-18	08-Jul-22	13546	5119821	$7,333,429	
HEX Photon Delivery System Procurement and Fabrication		**690**	**22-May-18**	**25-Feb-21**	**0**	**3337809**	**$3,739,494**	
HEX14290	Photon Delivery System Delay Due to Funding Profile - 6M	187	22-May-18	21-Feb-19	0	0	$0	SPP
HEX251961	HEX - Review Scope and Budget Prior to Mono and Non O	5	08-Aug-19	14-Aug-19	0	0	$0	SPP
HEX14220	HEX - PDR, Status and FAT visits to Vendors	360	16-Sep-19	25-Feb-21	0	45000	$52,992	SPP
HEX14420	Procure Vacuum Pump and Gauge Controllers and Cables	60	06-Jul-20	28-Sep-20	0	211902	$237,118	SPP
Laue Mono		**503**	**22-Feb-19**	**25-Feb-21**	**0**	**819607**	**$917,632**	
HEX251541	Prepare Procurement Documentation	30	22-Feb-19	04-Apr-19	0	0	$0	SPP
HEX251611	Accept Req at PPM	1	05-Apr-19	05-Apr-19	0	0	$0	SPP
HEX251551	Prepare and submit RFP	27	05-Apr-19	13-May-19	0	0	$0	SPP
HEX251561	Receive Proposals	25	14-May-19	18-Jun-19	0	0	$0	SPP
HEX251571	Evaluate Proposals	25	19-Jun-19	24-Jul-19	0	0	$0	SPP
HEX251581	Negotiate with Offerors	10	25-Jul-19	07-Aug-19	0	0	$0	SPP
HEX251591	Prepare & Approve Contract Package	25	08-Aug-19	12-Sep-19	0	0	$0	SPP
HEX251601	Contract Award	1	13-Sep-19	13-Sep-19	0	0	$0	SPP
HEX14100	1 Laue mono	360	16-Sep-19	25-Feb-21	0	819607	$917,632	SPP
Non Optics Components		**503**	**22-Feb-19**	**25-Feb-21**	**0**	**1921300**	**$2,151,087**	
HEX251621	Prepare Procurement Documentation	30	22-Feb-19	04-Apr-19	0	0	$0	SPP
HEX251631	Accept Req at PPM	1	05-Apr-19	05-Apr-19	0	0	$0	SPP
HEX251641	Prepare and submit RFP	27	05-Apr-19	13-May-19	0	0	$0	SPP
HEX251651	Receive Proposals	25	14-May-19	18-Jun-19	0	0	$0	SPP
HEX251661	Evaluate Proposals	25	19-Jun-19	24-Jul-19	0	0	$0	SPP
HEX251671	Negotiate with Offerors	10	25-Jul-19	07-Aug-19	0	0	$0	SPP
HEX251681	Prepare & Approve Contract Package	25	08-Aug-19	12-Sep-19	0	0	$0	SPP
HEX251691	Contract Award	1	13-Sep-19	13-Sep-19	0	0	$0	SPP
HEX14200	Non-optics components	360	16-Sep-19	25-Feb-21	0	1921300	$2,151,087	SPP
White Beam Shutters		**323**	**17-Jun-19**	**28-Sep-20**	**0**	**340000**	**$380,664**	
HEX251701	Prepare Procurement Documentation	30	17-Jun-19	29-Jul-19	0	0	$0	SPP
HEX251711	Accept Req at PPM	1	30-Jul-19	30-Jul-19	0	0	$0	SPP
HEX251721	Prepare and submit RFP	27	30-Jul-19	05-Sep-19	0	0	$0	SPP
HEX251731	Receive Proposals	25	06-Sep-19	10-Oct-19	0	0	$0	SPP
HEX251741	Evaluate Proposals	25	11-Oct-19	18-Nov-19	0	0	$0	SPP
HEX251751	Negotiate with Offerors	10	19-Nov-19	04-Dec-19	0	0	$0	SPP
HEX251761	Prepare & Approve Contract Package	25	05-Dec-19	10-Jan-20	0	0	$0	SPP
HEX251771	Contract Award	1	13-Jan-20	13-Jan-20	0	0	$0	SPP
HEX14210	2 Special White Beam Shutters	180	14-Jan-20	28-Sep-20	0	340000	$380,664	SPP
HEX Photon Delivery System Installation and Test		**778**	**30-May-19**	**08-Jul-22**	**13066**	**2500**	**$1,551,154**	
HEX251531	HEX - Engineering and Installation Oversight	778	30-May-19	08-Jul-22	4979	0	$655,709	SPP
HEX14230	HEX - Beamline Technician Effort	579	14-Jan-20	05-May-22	3706	0	$378,033	SPP
HEX14130	Special White Beam Shutters Installation and Testing	10	29-Sep-20	13-Oct-20	60	0	$7,264	SPP
HEX14190	HEX - Photon Delivery System Installation and Test Labor	232	29-Sep-20	01-Sep-21	2313	0	$278,665	SPP
HEX14440	Additional Rigger Hours	232	29-Sep-20	01-Sep-21	748	0	$99,743	SPP
HEX251971	HEX - EEI Labor for Electrical Inspection	232	29-Sep-20	01-Sep-21	0	0	$0	SPP
HEX25380	HEX - PPE Costs (Safety shoes, Glasses etc.)	5	14-Oct-20	20-Oct-20	0	2500	$2,995	SPP
HEX14110	Non-optics components Installation and Testing	132	26-Feb-21	01-Sep-21	720	0	$73,568	SPP
HEX14140	Laue mono Installation and Testing	132	26-Feb-21	01-Sep-21	540	0	$55,176	SPP
HEX14180	HEX - All Beamline components testing complete	0		01-Sep-21	0	0	$0	SPP
HEX End Station Procurement and Fabrication		**250**	**17-Sep-20**	**16-Sep-21**	**0**	**1779512**	**$1,992,342**	



Summary

- **Optics:** HEX optics and endstations are extremely simple, optical design and simulation is quite advanced
- **Technical feasibility:** Many technical challenges overcome. BNL expertise with high-energy x-ray optics. Future development in detector, optics, and new science directions are easily incorporated due to white-beam/removable optics concept.
- **Heat load** is large, but manageable.
- **The scope, cost, schedule, risks** are well-understood.

Thanks To

- **NSLS-II** Andrew Broadbent, Mike Lucas, Eric Dooryhee, David Sprouster, Milinda Abeykoon, Ken Evans-Lutterodt, Sanjit Ghose, Wah-Keat Lee, Hengzi Wang, Oleg Tchoubar, Weiming Guo, Steve Hulbert, Pete Siddons, Lonny Berman, Sushil Sharma, Hui Zhong
- **User Community**
  - Esther Takeuchi, Feng Wang, Can Erdonmez
  - Mark Croft, Thomas Tskakalakos, Koray Akdogan, and Alex Ignatov
  - John Parise, Don Weidner, Lars Elm, Jiuhua Chen, Xinguo Hong, Avraham Dilmanian
  - Dan Steingart, Josh Gallaway
  - Yan Gao, Juliana Cernatescu
  - Nick Simos, Lynne Ecker
- **Advisers** Ke Yang, Cai Quan, Michael Drakopoulos, John Okasinski, Jon Almer, Shastri Sarvjit, Xianbo Shi, Dean Chapman,Tomasz Wysokinski, Peter Ko, Daniel Hausermann, William Thomlinson
- **Management** Qun Shen, Ron Pindak, Paul Zschack, Erik Johnson, Jim Misewich, and John Hill
- **NSLS-II CAMs** Greg Fries, Chris Stebbins, Timur Shaftan, Steve Hulbert, Toshi Tanabe, Charles Hetzel, Richard Farnsworth, Zhijian Yin, Ed Haas, John Gosman, George Ganetis, Chris Amundsen, Bernard Kosciuk, Raj Gutta, Mo Benmerrouche, Lori Stiegler, Joe Zipper