Thoughts on HEX Endstations

HEX PDR Meeting 4/26/2018

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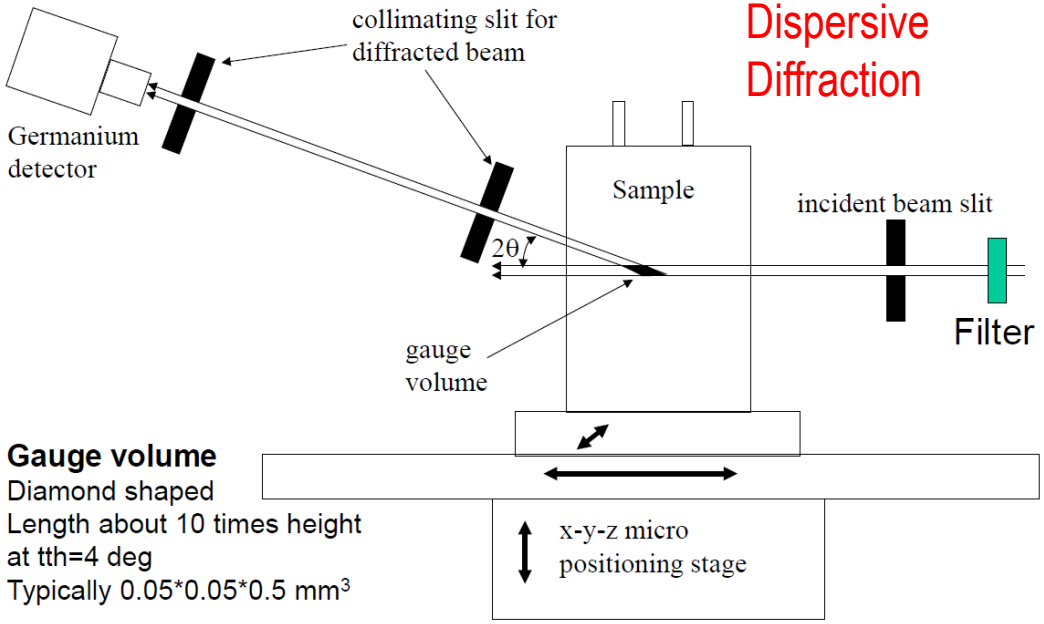
Outline

- Beamline Layout
- Endstations
  - Design and specification for three techniques
    - EDXD
    - Imaging
    - ADXD
- Milestones and summary

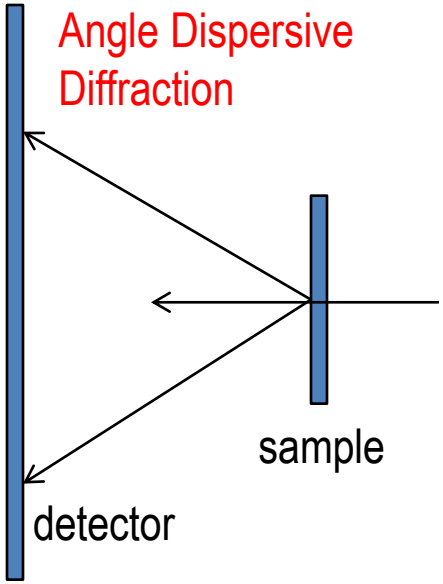
Three High-energy Techniques Under One Roof

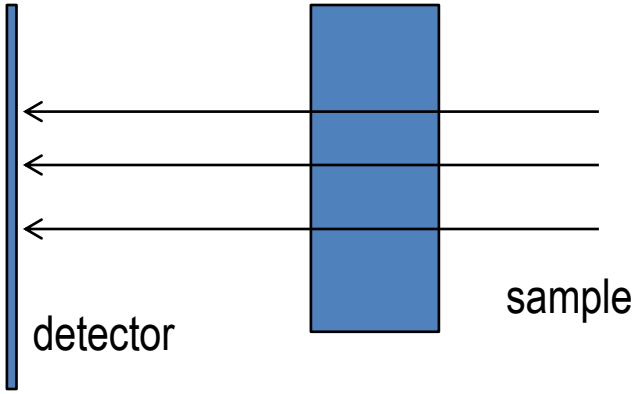
Energy Dispersive Diffraction



Gauge volume
Diamond shaped
Length about 10 times height at tth=4 deg
Typically 0.05*0.05*0.5 mm^3

Angle Dispersive Diffraction





Imaging

HEX Center Branch Specifications

TECHNIQUE(S):

Energy Dispersive X-ray Diffraction

Angle Dispersive X-ray Diffraction

Imaging with absorption or phase contrast

SOURCE:

Superconducting wiggler, SCW70, 4.3 T, 7 cm period, ~1 m length

ENERGY RANGE:

20-200 keV (EDXD)

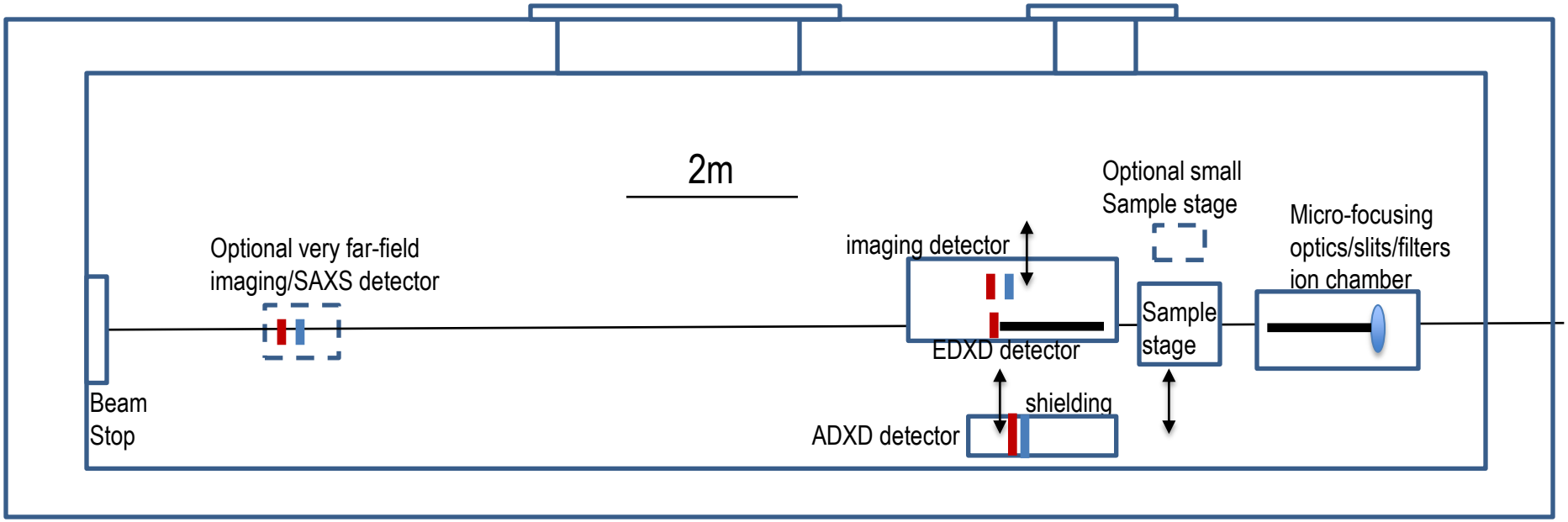
ADXD using imaging beam (30-150 keV)

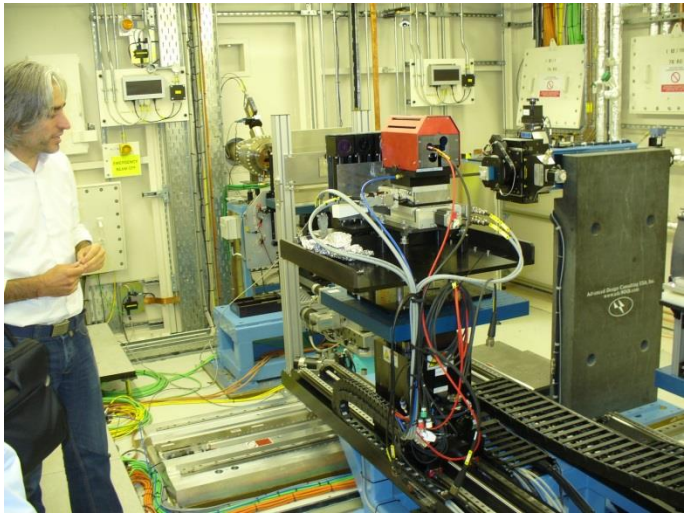
Imaging (30 – 150 keV)

SPATIAL RESOLUTION:

~1 μm imaging; 10 μm EDXD, 10 μm (micro-focusing)-0.5 mm ADXD

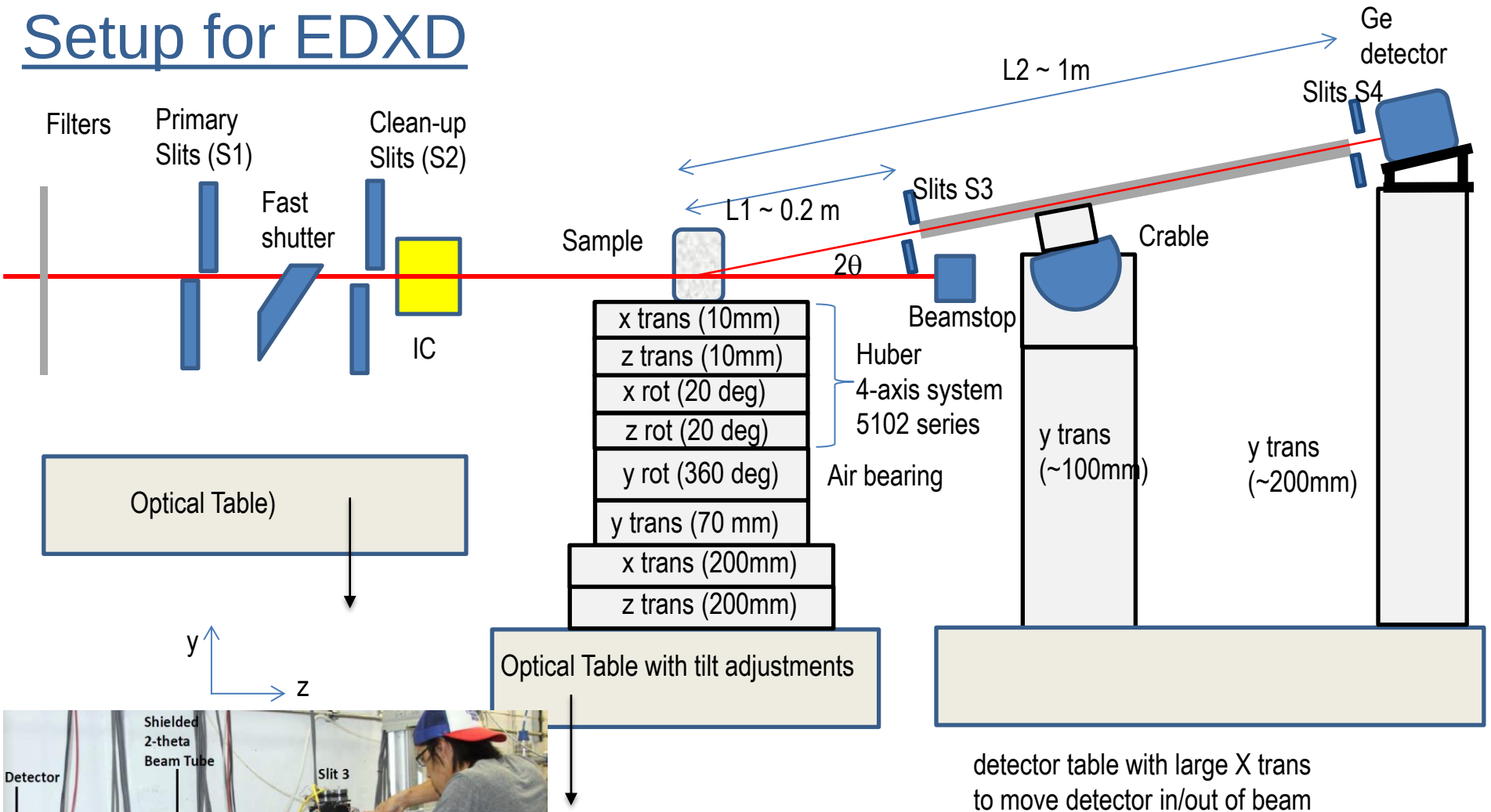
Endstation F in External Building

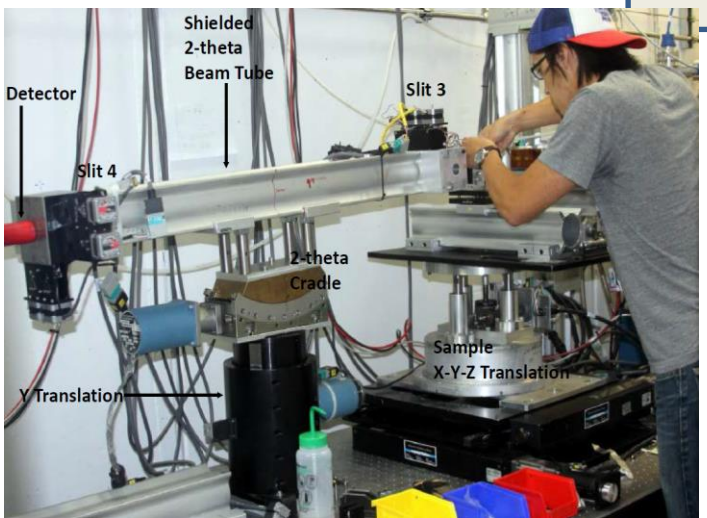




Endstation F in External Building

Setup for EDXD





detector table with large X trans to move detector in/out of beam (shared w/imaging)

Specification for Beam Conditioning

Component	Specification	Notes
Filter Assembly	SiC, 1, 2, 4 mm, Copper 0.1, 0.2, 0.4 mm Vacuum compatible	Water-cooling required
4-jaw Slits1 &2	0-25 mm (V) x 0-120 mm (H) 1 micron resolution 10 mm Tungsten blade Slit 1 is vacuum compatible	Water-cooling required
Ion Chamber	0-25 mm (V) x 0-120 mm (H) area 60 mm sensitive depth Thin (~50 microns) Aluminum window	IC (with air) response is 0.54 nA for 10^9 ph/s @ 80 Kev We have 2 segmented IC from X15A
Fast Shutter	25 mm (V) x 120 mm (H) 10 ms response time	
Micro-focusing optics	K-B mirrors (0.5 m length for each mirror) or saw-tooth optics 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
Beam conditioning table	1 m width x 3 m length, at 1 m nominal height 0-100 mm vertical adjustment to switch between monochromatic beam and white beam, 1 micron resolution	

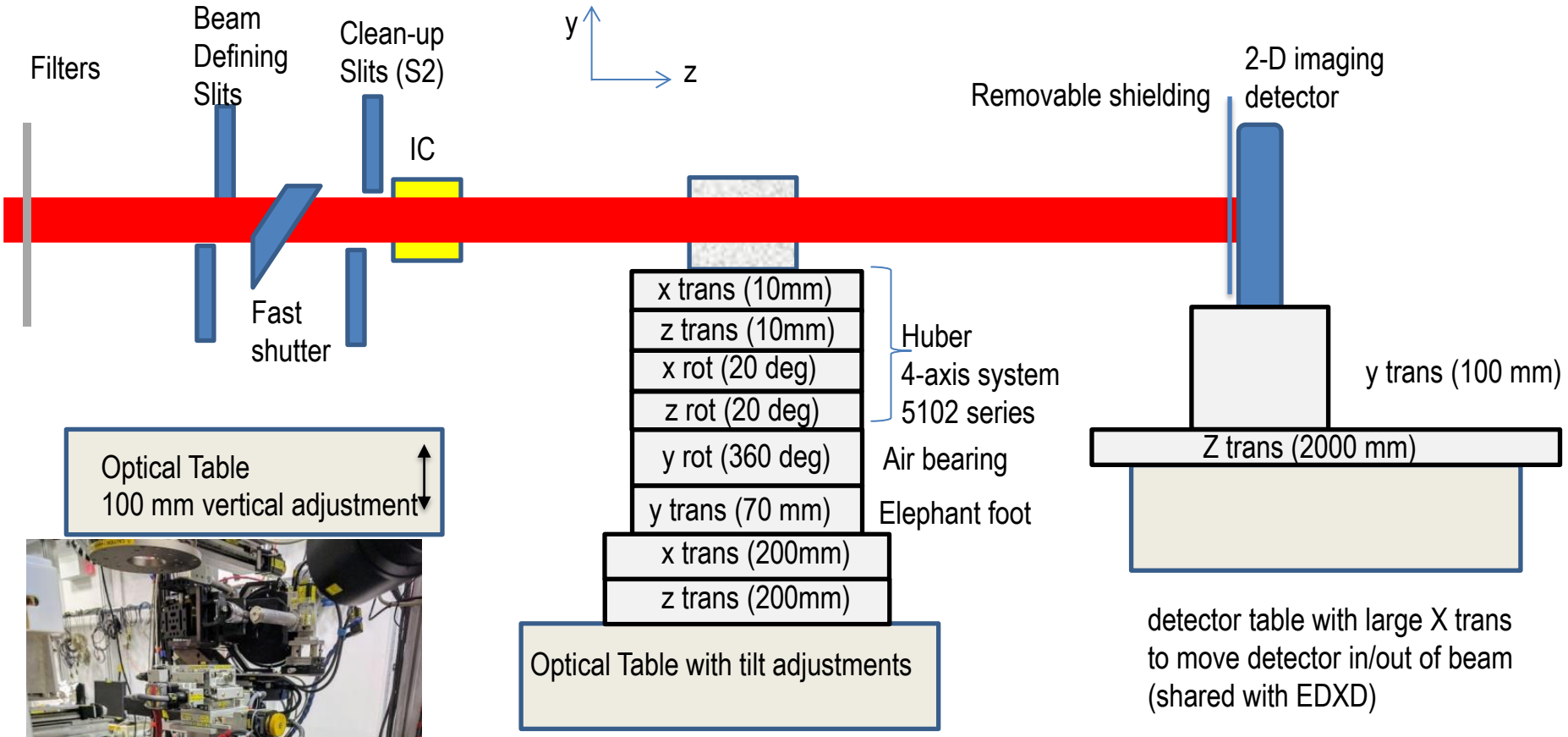
Specification for Sample Stack

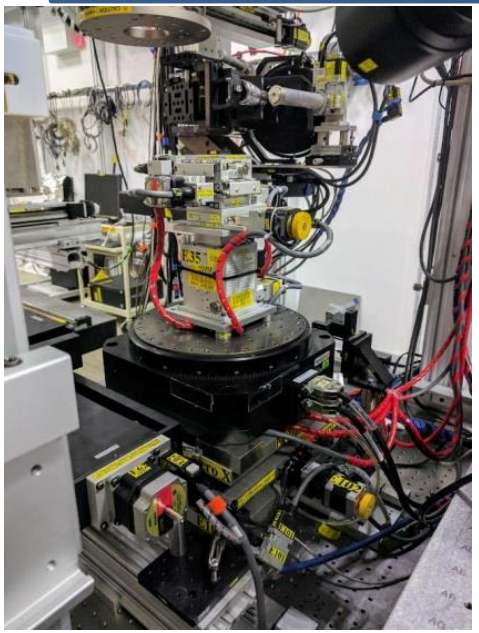
Component	Specification	Notes
X-Z Translation on X-Z Cradle	+-10 mm translation range with 1 micron resolution +- 20 degrees rotation with 0.001 deg. resolution 50 kg load	Reference Huber 5102
360 deg. goniometer for CT	360 deg. rotation range with 0.001 deg. resolution 10 rev./s maximum rotation speed 75 kg load	Reference ESRF ID-19 or APS 2-BM CT rotation air bearing
Y translation	70 mm range, 1 micron resolution 100 kg load	Reference NSLS elephant foot
X-Z Translation	200 mm range, 1 micron solution 150 kg load	
Sample table	0.5 m width x 0.5 m length, at 0.75 m nominal height 0-100 mm vertical adjustment to switch between monochromatic beam and white beam Tilt adjustment +- 1 deg. with 0.001 deg. resolution, needed for alignment of CT rotation axis 200 kg load	Tilt adjustment can be achieved through kinematic mount of 3 vertical jacks

Specification for EDXD

Component	Specification	Notes
4-jaw Slits3 &4	0-10 mm (V) x 0-10 mm (H) 1 micron resolution 10 mm Tungsten blade	In-air
X95 link between slits 3&4	Constructed of X95 of 800 mm length End machined to mount slits Bore hole (~50 mm diameter) lined with 5mm thick lead	
Y translation	100 mm range, 1 micron resolution 50 kg load 1 micro-radians angular stability	Prefer design with center jack and large (>100 mm) footprint to promote angular stability
Cradle for 2-theta arm	+-20 deg. range, 0.001 deg. resolution 30 kg load	
Detector jack	200 mm range, 10 micron resolution 30 kg load	
Detector angle tilt	0-10 deg. tilt adjustment 20 kg load	Kinematic mount or cradle
Ge detector 2 units	15 mm diameter sensitive area, 5 mm Ge thickness 20- 200 keV	Reference Canberra x-ray detector and XIA MCA
EDXD + Imaging table	1 m width x 3 m length, at 1 m nominal height Large (0-2m) x Translation to move detector in/out of beam. 200 kg load	Height adjustment is desirable

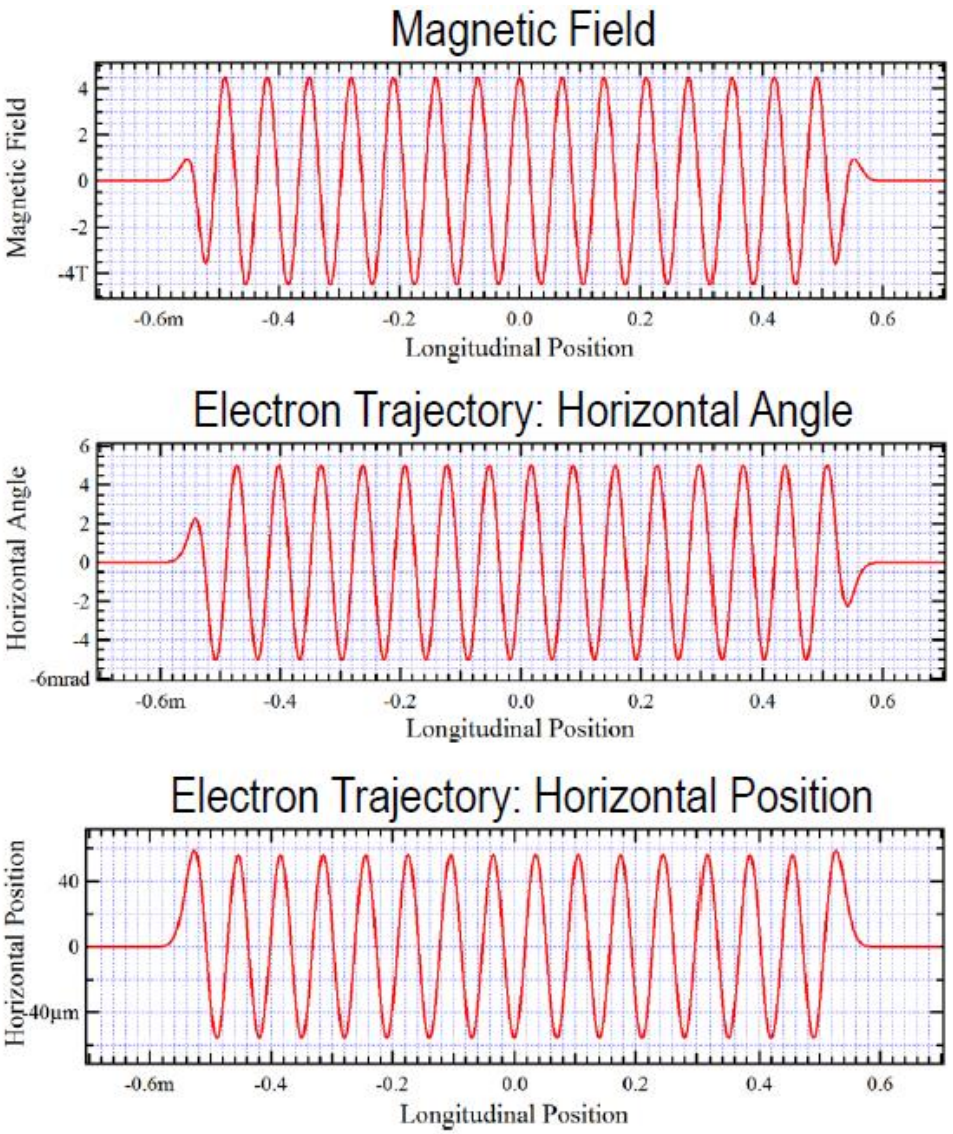
Setup for Imaging



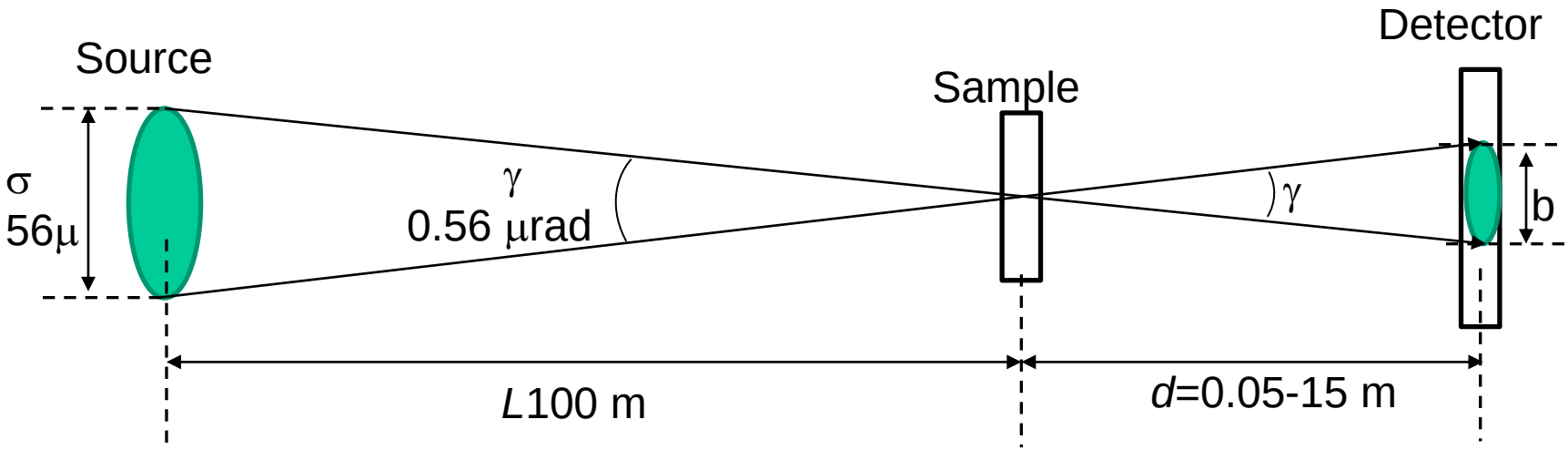


SCW70 Source Size

- Electron σ_{x_ebeam}=41μ, σ_{y_ebeam} =3μ
- Electron excursion is 107 μ. Assuming sine wave, $\sigma_{x\_excursion}$=107/2.8=38 μ
- Combined σ_x=56μ, σ_y=3μ
- Multiplying by 2.36 results in source size of **132 μ (H) by 7 μ (V) FWHM**.
- Horizontal source size dominates in imaging and focusing considerations



Propagation-based Phase Contrast



- For weak phase object: $I(x) \approx 1 + \frac{\lambda d}{2\pi}\phi''(x)$, ϕ is the phase of transmitted beam wavefront.
- Contrast increases with sample-detector distance *d*.
- Penumbral angle $\gamma = \sigma/L$ characterizes phase-contrast sensitivity of a beamline
- Image blurring due to source size $b = d\sigma/L$, want large source-sample distance *L*
- In the satellite station at *L*=100 m,
  - γ= 0.56 μrad RMS, 1.3 μrad FWHM,
  - b= 0.07μ - 20 μ FWHM. Note detector resolution is limited to about 1 μ.
- 0.05 m – 1 m d satisfy needs for most experiments from ESRF19ID and APS 2BM experience. Cracks, voids: < 0.5 m, Insects: < 1 m. Specify 0.05-2 m detector z
- Careful about wave-front distortion by SiC filters.

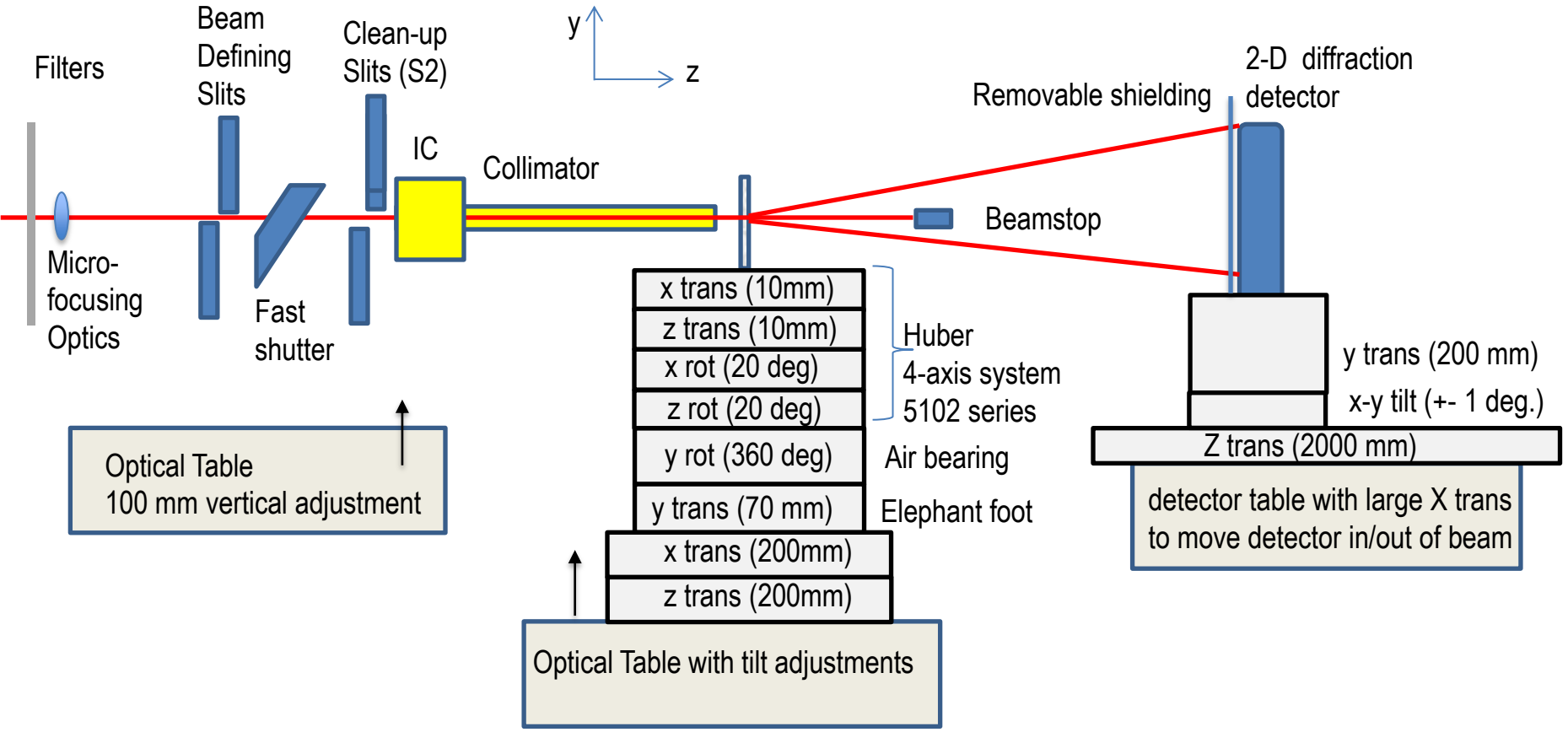
Specification for Imaging

Component	Specification	Notes
2-D Imaging detectors (large area)	20 mm (V) x 100 (H) sensitive area 30 keV – 150 keV 5 micron – 250 micron resolution	Reference ESRF 19-ID and IMBL modular imaging detector
2-D Imaging detector (high resolution)	20 mm (V) x 20 mm (H) sensitive area 30 keV-100 keV 1-5 micron resolution	Reference ESRF 19-ID and IMBL modular imaging detector
Y translation	70 mm range, 1 micron resolution 20 kg load	
Z translation	2m range, 10 micron resolution 30 kg load	
Table for far detector	0.5 m width x 1 m length, at 1 m nominal height 200 mm vertical translation to move detector in/out of beam	Optional
Table shared with EDXD	1 m width x 3 m length, at 1 m nominal height Large (0-2m) x Translation to inboard move detector in/out of beam. 200 kg load	Height adjustment is desirable

Imaging: Global context

Beamline	Average photon density (ph/s/mm^2/0.1%bw @ 60 keV	FWHM horizontal penumbra angle ($\sigma/L*2.35$)	Beam Size H X V (mm)	Energy Range (keV)
HEX	**1.3x10^{11}**	**1.3 μrad**	**100 x 20**	**30-150**
ESRF ID19 W	2x10^{11}	0.9 μrad (on-axis)	45 x 6	20-100
SPRING8 BL20XU@245 m	3x10^{11}	2.9 μrad	4 x 2	10-60
APS 32-ID @70 m (RHB)	1.6x10^{11}	4 μrad	13 x 2.5	10-60
APS BM @70 m	4.5x10^{9}	2.7 μrad	(70) x 8	10-60

Setup for ADXD



Specification for ADXD

Component	Specification	Notes
Collimator	XPD & PDF design	
Beam stop with embedded photo-diode	~ 2 mm diameter 5 mm Tungsten depth Remote control of +- 3 mm in x-y position	Reference PDF beam-stop design
ADXD flat panel detector	400 mm×400 mm active area, CsI phosphor coating 0.2mm pixel	Reference XPD & PDF detectors Will wait for technology to improve
Y translation	200 mm range, 1 micron resolution 40 kg load	Prefer design with center jack
Detector angle tilt	Around x (H) and y(V) axis +-1 deg. tilt adjustment, 0.001 deg. resolution 50 kg load	For alignment Facilitates changing between apertured beam and K-B focused beam
Z translation	2m range, 10 micron resolution 30 kg load	
ADXD table	0.5 m width x 2 m length, at 0.75 m nominal height Large (0-1.5m) x Translation outboard 200 kg load	Height and tilt adjustment is optional

Samples

	Al	Steel	Ni	Battery (NaMx)	Water	Max. spec.
Thickness for 5% transmission (cm)	8.0	2.0	1.5	6.0	20	20 cm
Weight assuming cube (kg)	1.3	0.06	0.03	0.43	8.0	50 kg

- Maximum sample size: dictated by absorption of x-rays.
- Assuming 150 keV x-ray, the highest usable median energy after the sample, and 10% transmission, the maximum sample thickness calculated.
- Specification for max. sample size is based on water. Max. weight of 50 kg accomodates sample environment.
- Door width/height: 2 m
- Sample mount: magnetic base kinematic mount: 2x2.45 inch

HEX Branches

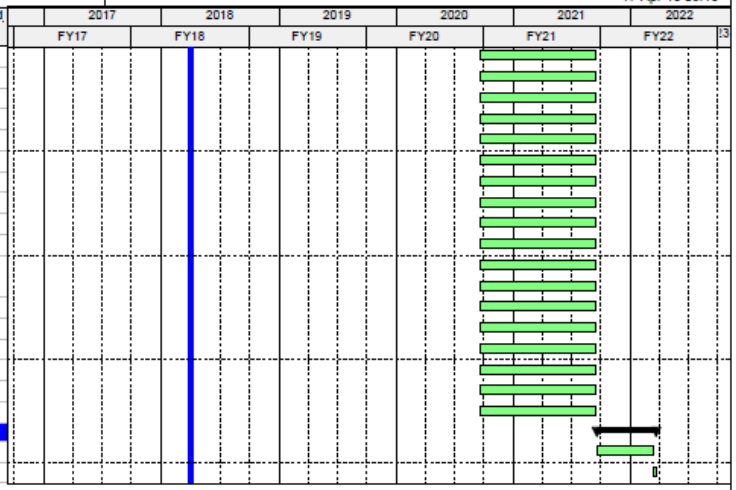
	Side branch	Center branch	White-beam branch
Technique	ADXD, PDF	EDRD, ADXRD, imaging, propagation-based phase contrast, small angle scattering, CT	EXRD
Beam size	0.5 mm x 0.5 mm	0.5 mm x 0.5 mm for diffraction 15 mm x 100 mm for imaging 10 microns x 10 microns for micro-focusing	5 mm x 5 mm
Flux/flux density (at 50 keV)	10^{12} ph/s for focused beam	10^{11} ph/s/mm^2 for imaging beam 10^{15}/ph/s/0.1%bw/mrad^2 for white beam 10^{13} ph/s for focused beam	10^{15}/ph/s/0.1%bw /mrad^2 for white beam
Resolution	0.5 mm	10 microns for EDXD 1 microns for Imaging 0.5 mm for ADXRD with unfocused beam 10 microns for ADXD with micro-focused beam	10 microns EDXD
Energy range (keV)	40-120	20-200 keV for white beam 30 – 150 keV for imaging and ADXD	20 – 200 keV white beam
Mode	Monochromatic	White/Monochromatic	White

Key Milestones

Milestone	Date
Conceptual Design Review	Oct-17
Preliminary Design Review	Apr-18
Final Design Review	May-19
Optical Components Ordered	Sep-19
End Station Components Ordered	Sep-20

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
HEX251331	Procure Micro-focusing optics (KB-mirror)	250	17-Sep-20	16-Sep-21	0	400000	$447,840	SPP
HEX251341	Procure EDXRD Sample Stage	250	17-Sep-20	16-Sep-21	0	48000	$53,741	SPP
HEX251351	Procure EDXRD Sample table	250	17-Sep-20	16-Sep-21	0	65000	$72,774	SPP
HEX251361	Procure EDXRD Detector Table (Stable)	250	17-Sep-20	16-Sep-21	0	75000	$83,970	SPP
HEX251371	Procure 2 Theta Cradle (Slit on each end)	250	17-Sep-20	16-Sep-21	0	47912	$53,642	SPP
HEX251381	Procure EDXRD Detector, single element Ge detector (eg	250	17-Sep-20	16-Sep-21	0	140000	$156,744	SPP
HEX251391	Procure EDXRD Detector, multielement Ge R&D project Pe	250	17-Sep-20	16-Sep-21	0	100000	$111,960	SPP
HEX251401	Procure Lead Wall, 1" Thick, Sliding on floor rails (costed b	250	17-Sep-20	16-Sep-21	0	12600	$14,107	SPP
HEX251411	Procure Imaging Sample Stage	250	17-Sep-20	16-Sep-21	0	63000	$70,535	SPP
HEX251421	Procure Imaging Sample Table	250	17-Sep-20	16-Sep-21	0	65000	$72,774	SPP
HEX251431	Procure Imaging Detector Table	250	17-Sep-20	16-Sep-21	0	75000	$83,970	SPP
HEX251441	Procure Imaging Y-Z stage for detector (2m horiz translatio	250	17-Sep-20	16-Sep-21	0	75000	$83,970	SPP
HEX251451	Procure Floor Rails	250	17-Sep-20	16-Sep-21	0	60000	$67,176	SPP
HEX251461	Procure Imaging Beam Conditioning equipment	250	17-Sep-20	16-Sep-21	0	93000	$104,123	SPP
HEX251471	Procure ADXRD detector	250	17-Sep-20	16-Sep-21	0	100000	$111,960	SPP
HEX251481	Procure Detector translation stage (move between EDXRD	250	17-Sep-20	16-Sep-21	0	75000	$83,970	SPP
HEX251491	Procure Imaging Detectors	250	17-Sep-20	16-Sep-21	0	260000	$291,096	SPP
HEX251501	Procure Beam Stop	250	17-Sep-20	16-Sep-21	0	25000	$27,990	SPP
HEX End Station Installation and Test		**125**	**17-Sep-21**	**22-Mar-22**	**480**	**0**	**$50,439**	
HEX14170	G Endstation & Detector Installation and Testing Placeholde	120	17-Sep-21	15-Mar-22	480	0	$50,439	SPP
HEX14240	HEX - All End Station Installation & Testing Complete	5	16-Mar-22	22-Mar-22	0	0	$0	SPP



Summary

- **Endstations:** HEX endstations are extremely simple. Design and simulation of endstations for the three techniques are quite advanced
- **Technical feasibility:** No major technical challenges. BNL expertise with high-energy x-ray optics and detectors. Future development in detector, optics, and new science directions are easily incorporated due to white-beam concept.

Thanks To

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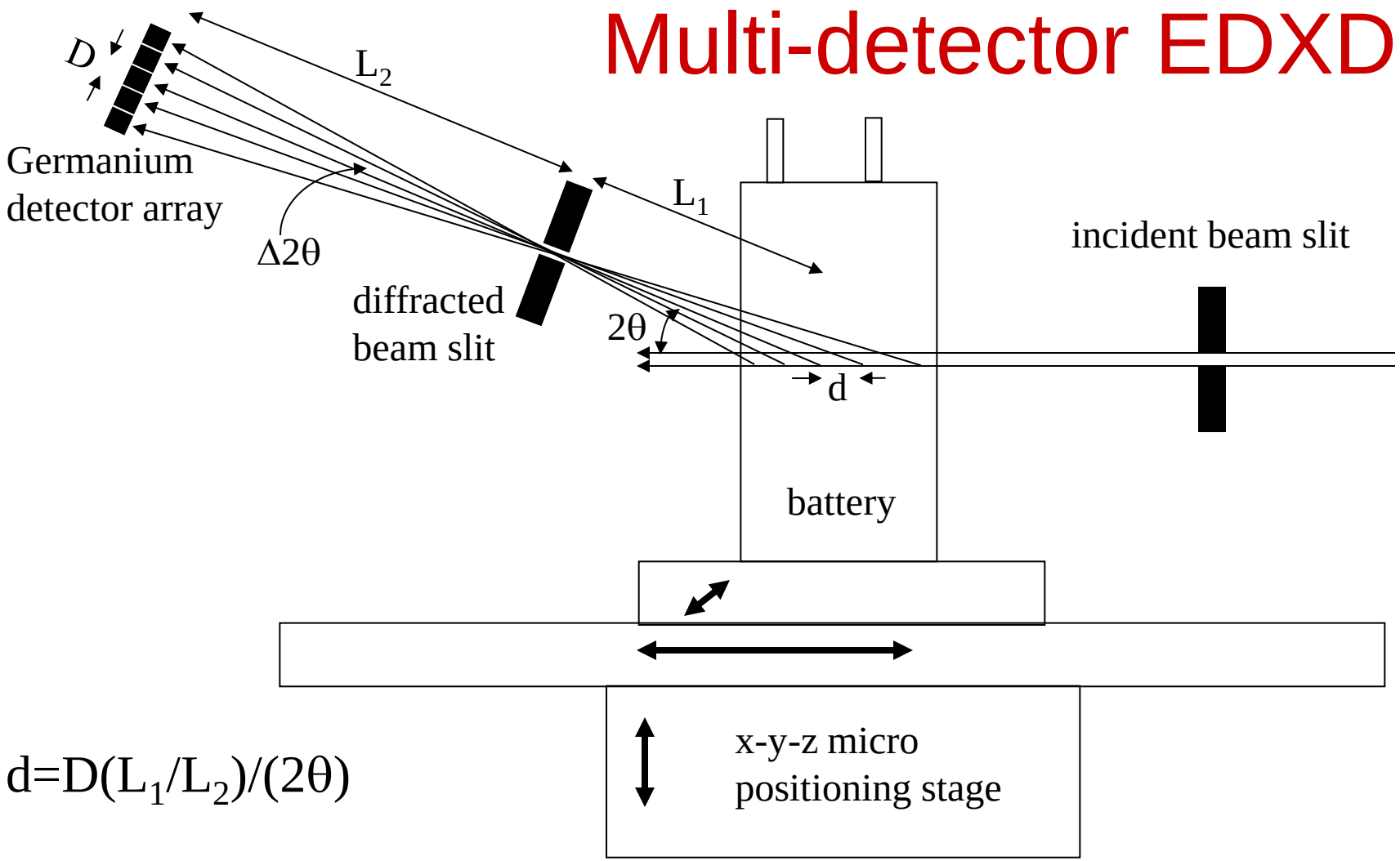
Multi-detector EDXD



$$d=D(L_1/L_2)/(2\theta)$$

- Each detector has different two-theta: Normalization of spectra and attenuation correction for quantitative phase analysis
- Construction of calibration sample having similar size and attenuation as the real sample

Specification for Multi-detector

design parameter	Quantity	Notes
d-spacing coverage	1.2 – 3.6 Å	
x-ray energy (E)	50 – 250 keV	60-150 energy range with flux above 10^9 ph/s/mm^2/keV
Two-theta angle (2θ)	4 degrees	Variable between 2 and 6 degrees to allow other d-spacing coverage
Two-theta variation between detector elements (Δ2θ/2θ)	< 20%	
Sample to diffraction slit (L_1)	0.2 m	
Sample to detector (L_1+L_2))	3 m	
Energy variation between detector elements for the same d-spacing (ΔE /E)	< 20%	
Detector pixel size	Minimum 0.25 mm (D) in plane, 10 mm out of plane	Smaller in-plane detector pixel size results in higher Z resolution along the x-ray beam
Number of detector elements (n)	160	
Detector size (D)	40 mm in place, 10 mm out of plane	
Sample coverage along beam direction (nd)	40 mm	
Resolution along beam (d)	0.25 mm	
resolution perpendicular to the beam	1-50 microns	Defined by the incident beam slit. Can be very small subject to counting time limitations