Energy Dispersive EXAFS
at
Diamond Light Source

Sofia Diaz-Moreno
Diamond Light Source

Harwell Science and Innovation Campus

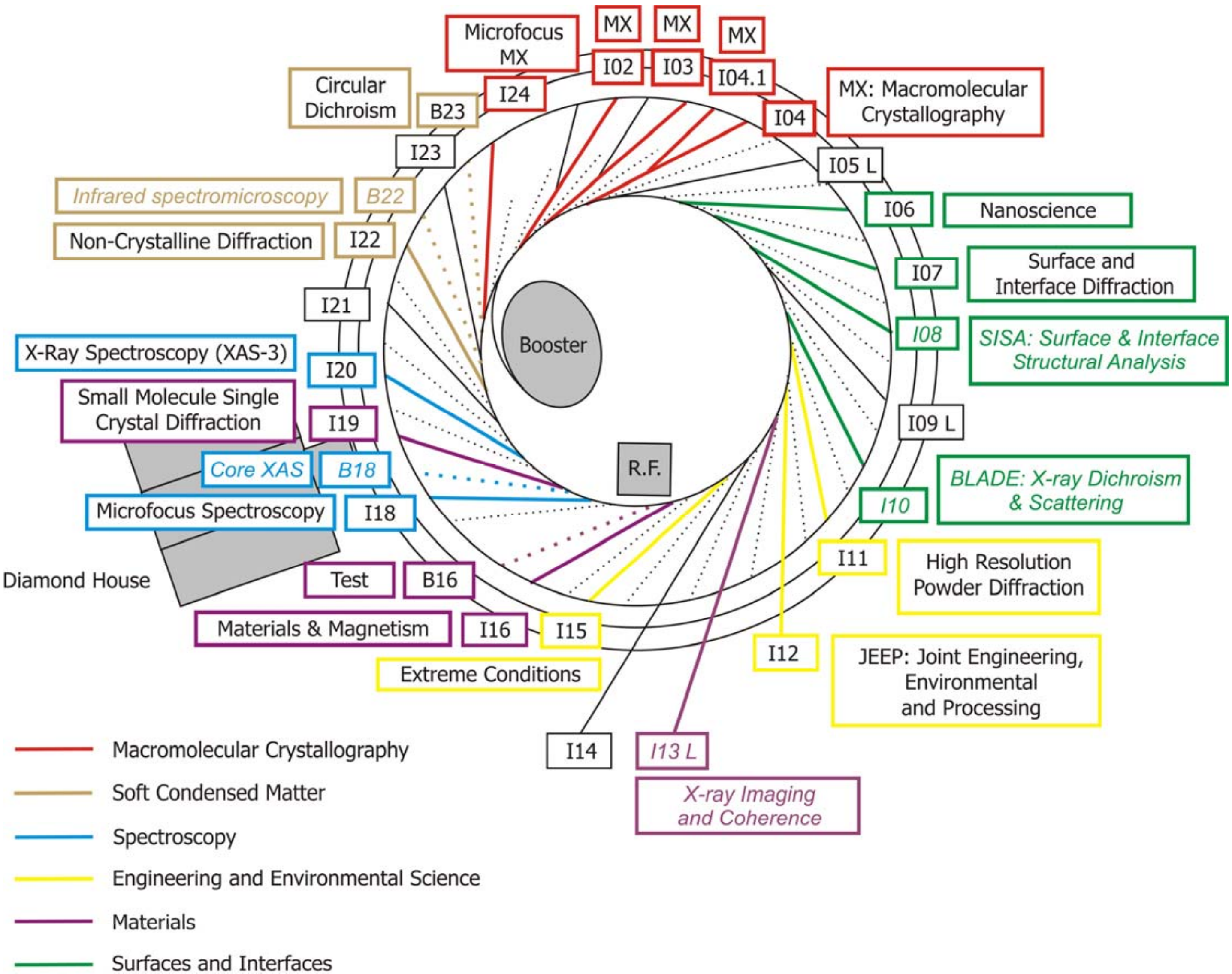
Central Laser Facility

diamond

ISIS Facility (Neutrons)

diamond parameters

Ring energy	3.0 GeV
Circumference	561.6 m
Ring diameter	235 m
Electron beam current	300 mA (500 mA)
Life time of the photon beam	10 hours
Emitance (horizontal)	2.7 nm-rad
Emitance (vertical)	0.03 nm-rad


Microfocus MX
MX
MX
MX
I02
I03
I04.1
Circular Dichroism
B23
I24
MX: Macromolecular Crystallography
I04
I23
I05 L
Infrared spectromicroscopy
B22
I06
Nanoscience
Non-Crystalline Diffraction
I22
I07
Surface and Interface Diffraction
I21
I08
SISA: Surface & Interface Structural Analysis
Booster
X-Ray Spectroscopy (XAS-3)
I20
Small Molecule Single Crystal Diffraction
I19
I09 L
R.F.
Core XAS
B18
BLADE: X-ray Dichroism & Scattering
I10
Microfocus Spectroscopy
I18
I11
High Resolution Powder Diffraction
Diamond House
Test
B16
Materials & Magnetism
I16
I15
I12
JEEP: Joint Engineering, Environmental and Processing
Extreme Conditions
I14
I13 L
X-ray Imaging and Coherence
Macromolecular Crystallography
Soft Condensed Matter
Spectroscopy
Engineering and Environmental Science
Materials
Surfaces and Interfaces

The history…

England has a long tradition in using dispersive XAS, mainly in time resolved activities.

The beamline used for this sort of experiments was station 9.3 at Daresbury Laboratory. This was a shared beamline with scanning EXAFS.

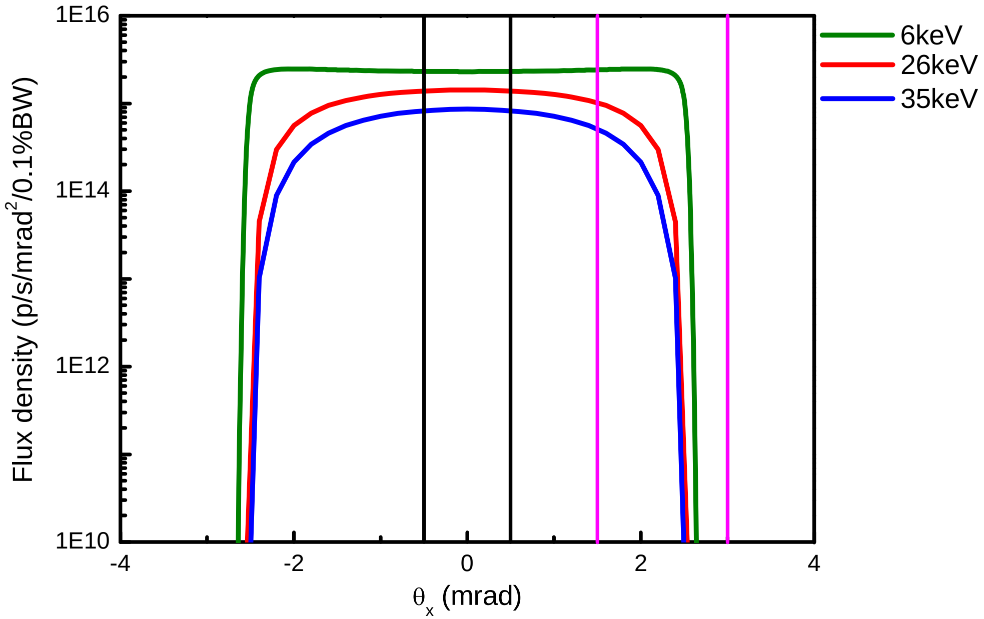
Within this context, I20 was proposed:

an instrument optimized for scanning EXAFS and dispersive XAS.

Technical challenges?

Proposed alternative (1)

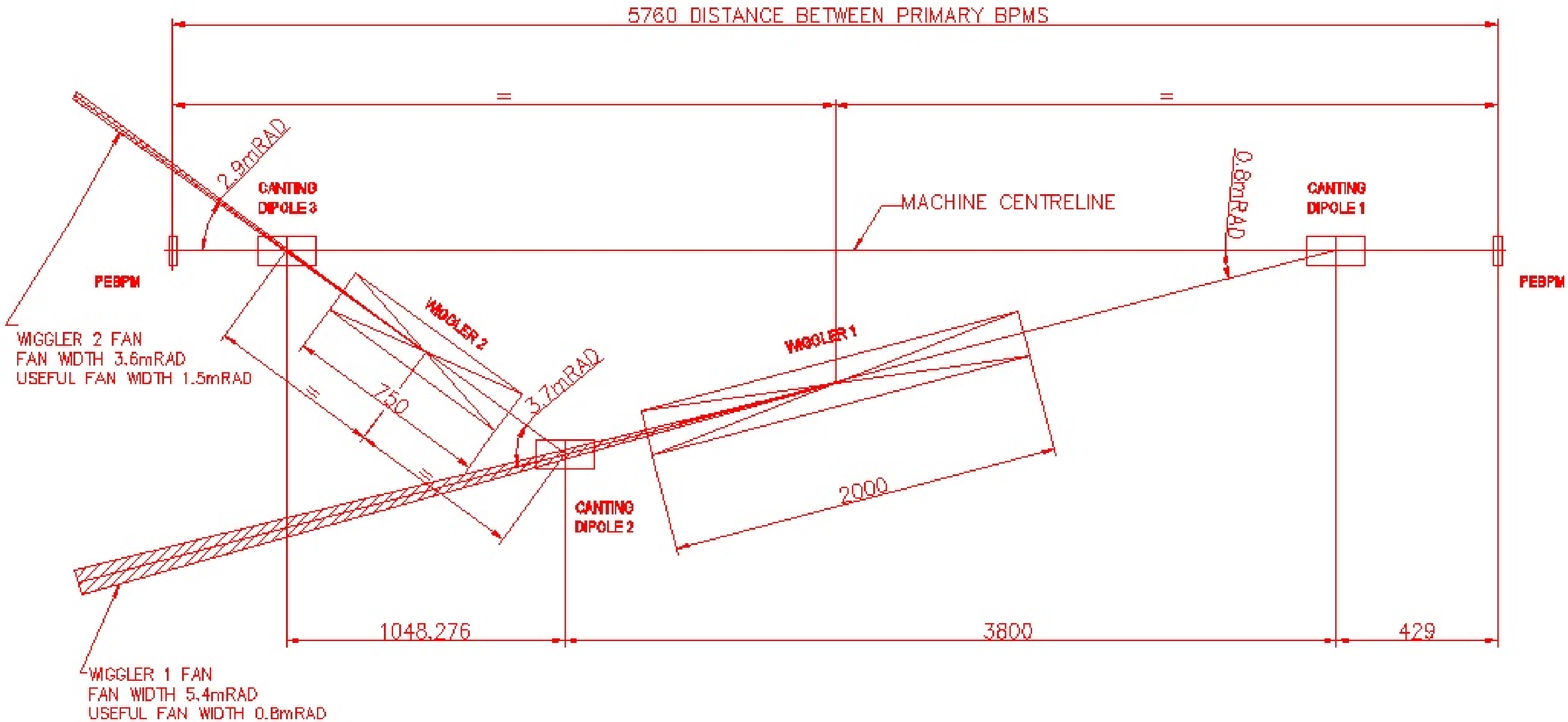
To use the broad horizontal fan of X-ray emission of the wiggler to build two separate beamlines: the central portion of the fan for the scanning EXAFS beamline and a side portion for the dispersive XAS.



The dispersive branch, located on the side of the radiation fan, is more prone to instabilities and in addition, the source size would be large.

Proposed alternative (2)

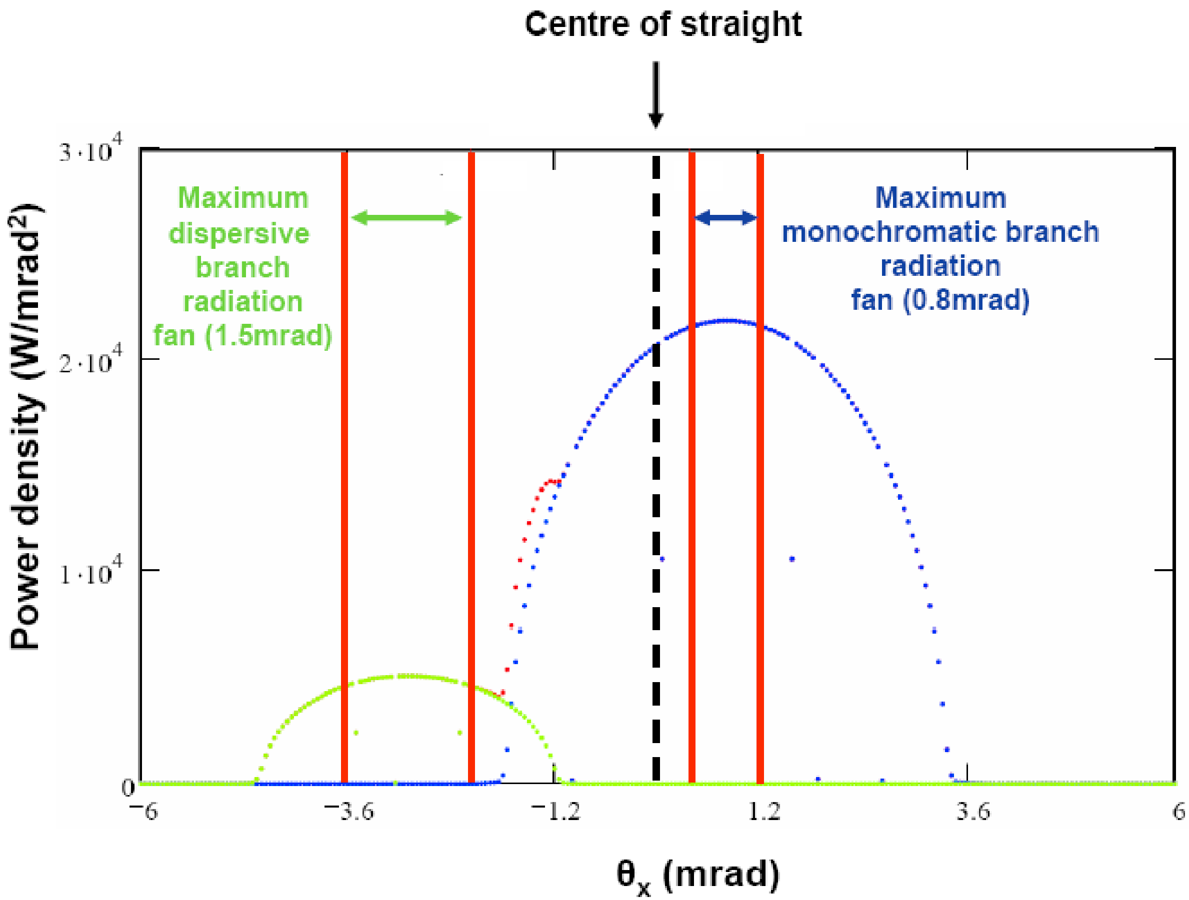
The second alternative is to use two different sources (wigglers) in a canted configuration.



Several restrictions on the choice of the dispersive wiggler.

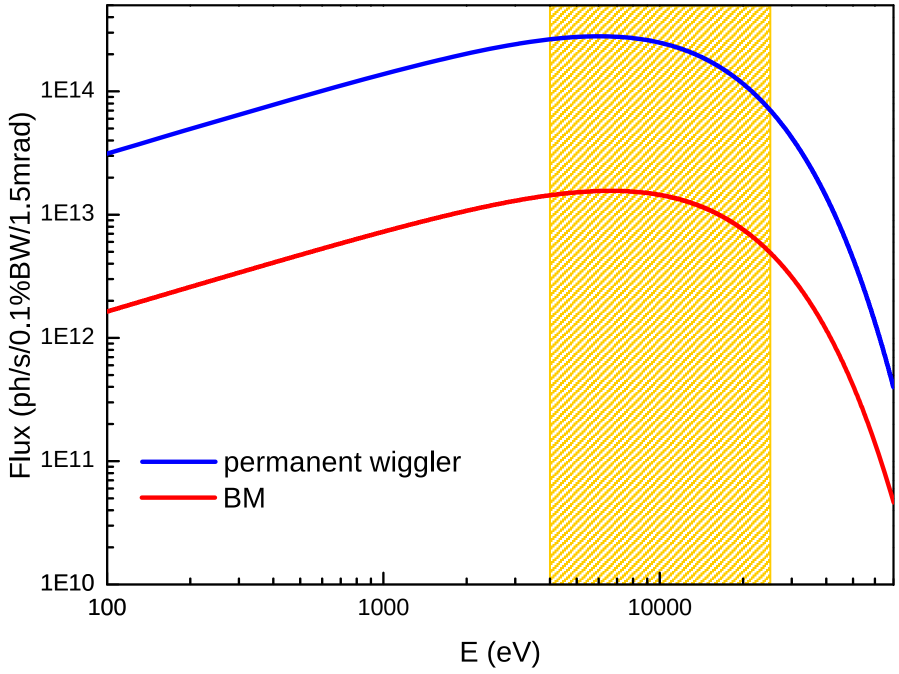
Proposed alternative (2)

Power distributions have been calculated at 500mA for W1 and W2. The canting angles need to allow full separation of both radiation fans.



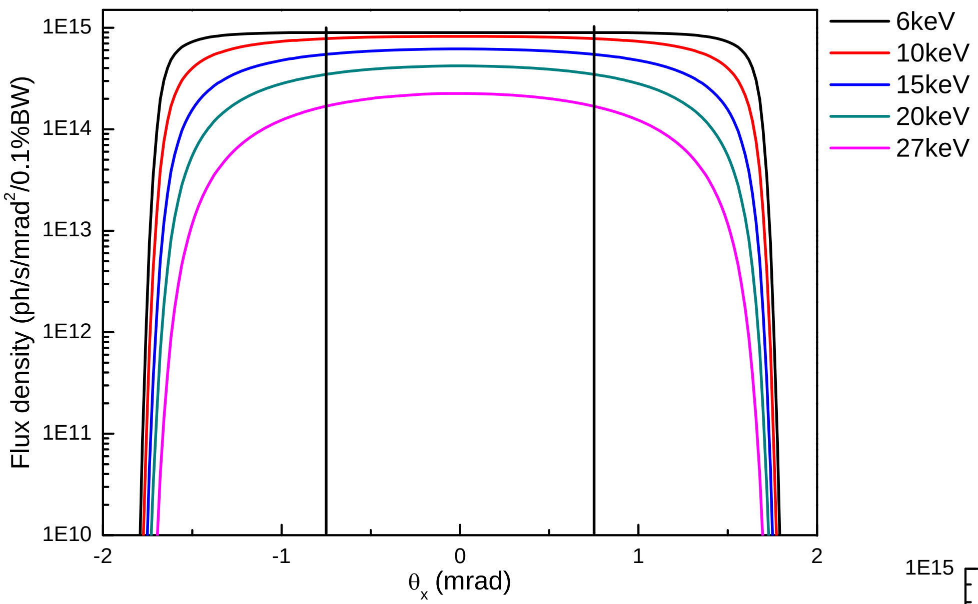
Source chosen

The comparison of flux delivered by the chosen permanent wiggler for EDE and a typical diamond bending magnet through the same aperture (1.5mrad) shows that the wiggler provides around an order of magnitude more flux across the entire operating energy range.



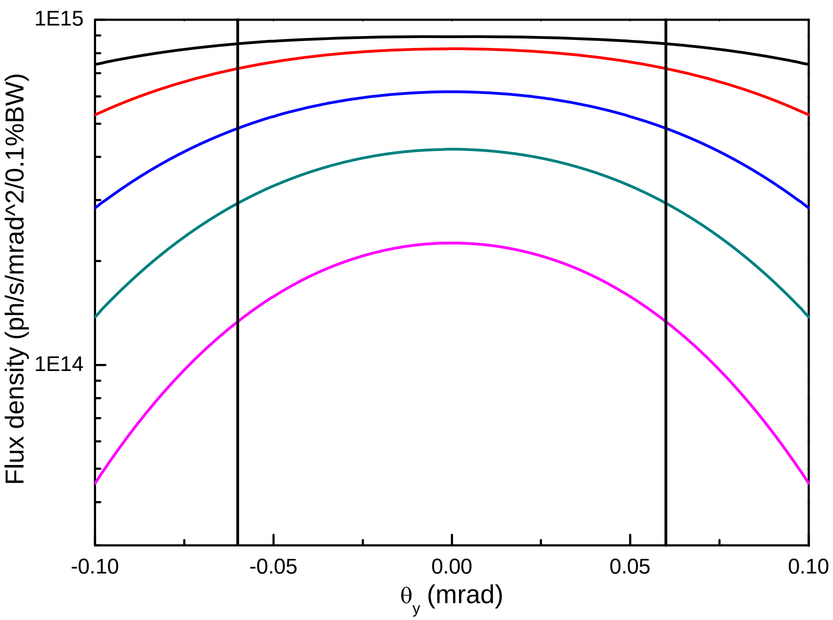
How flat is the emission?

Source chosen

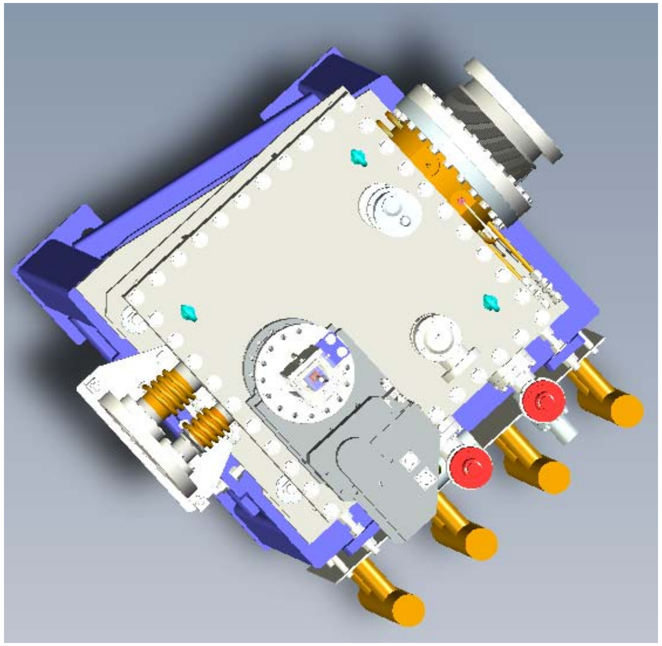


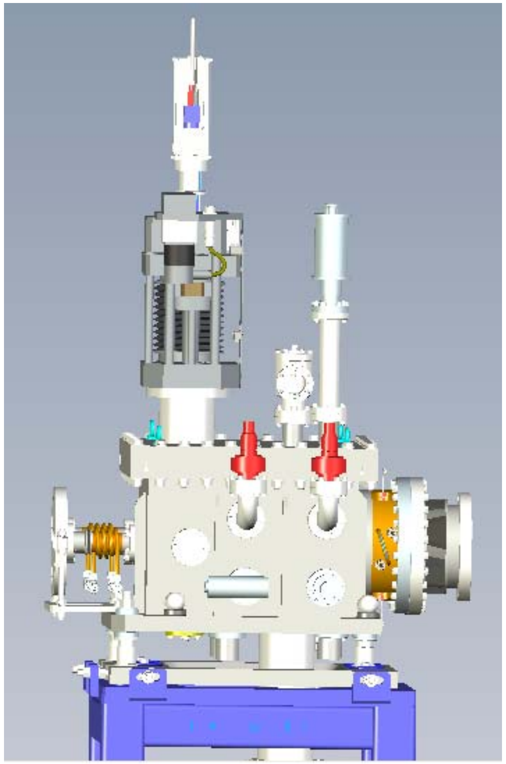
Horizontal angular emission for EDE wiggler at different energies

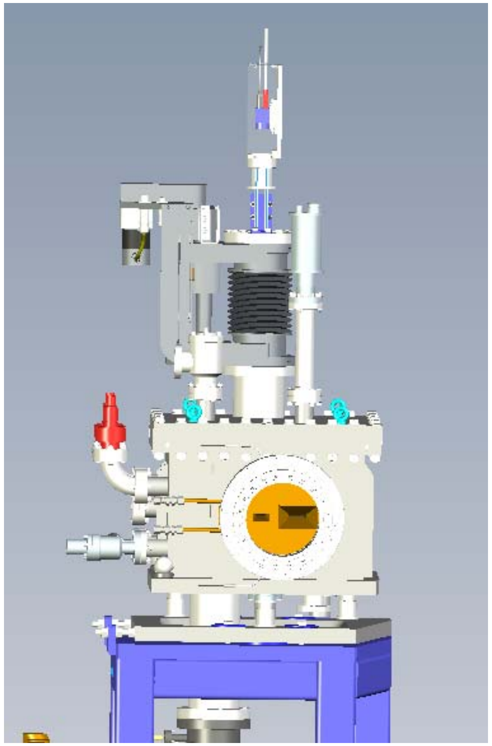
Vertical angular emission for EDE wiggler at different energies



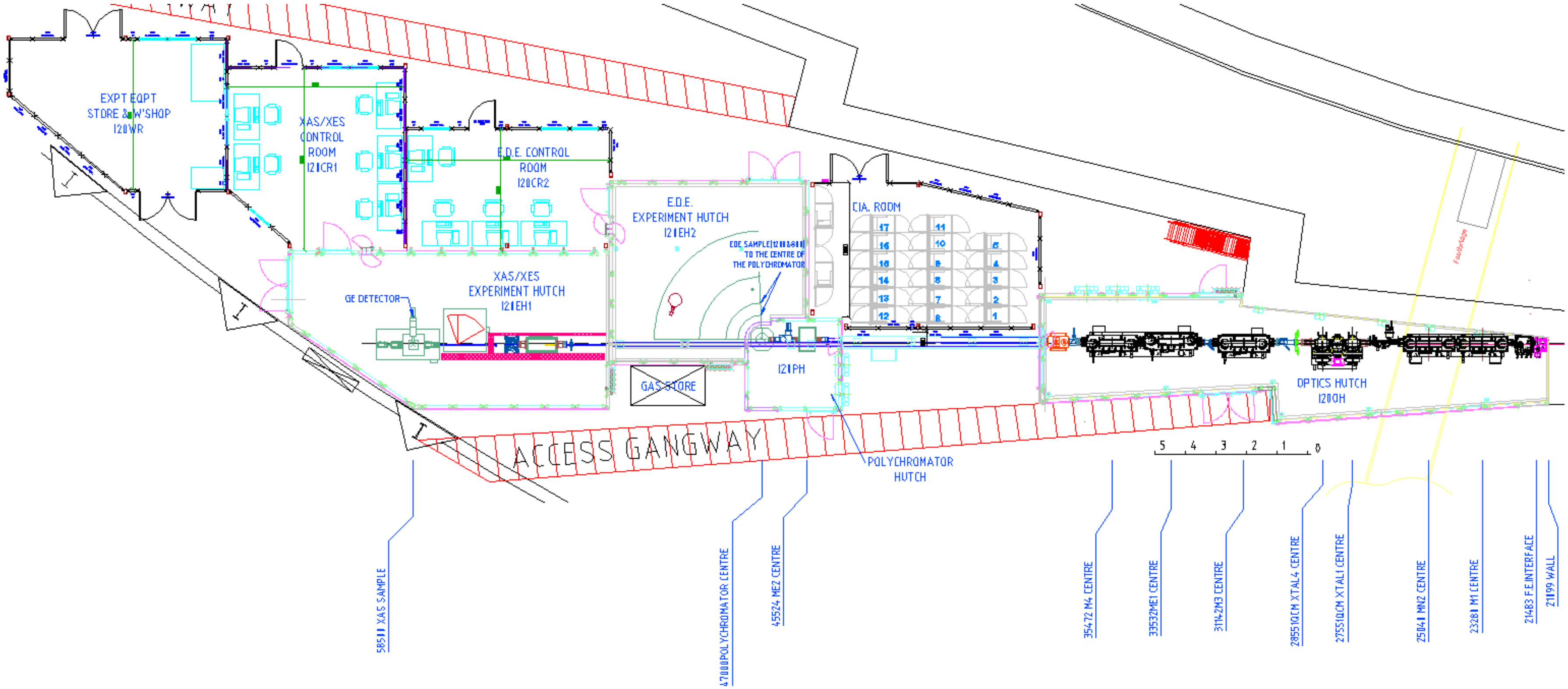
First element: collimator





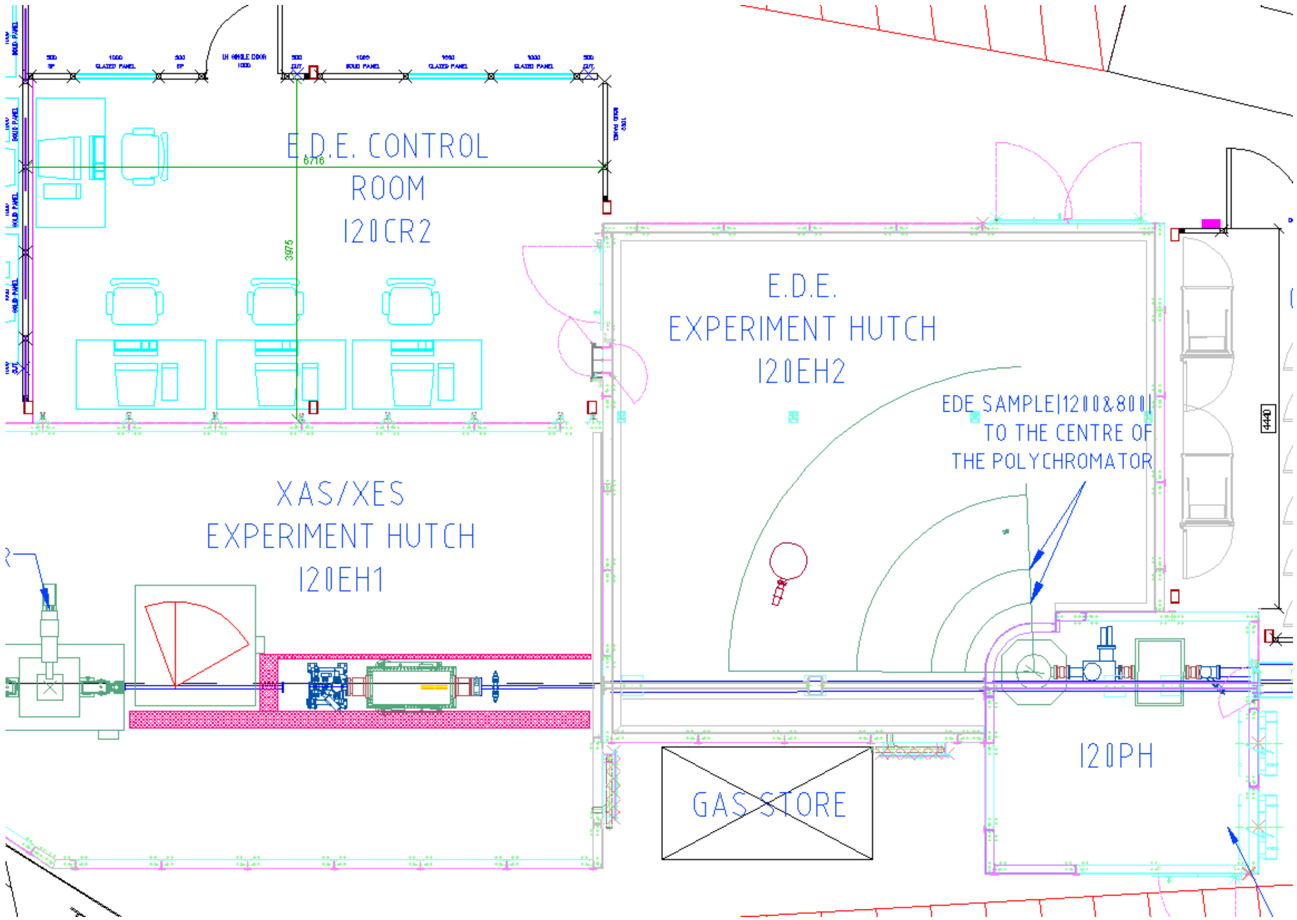


I20 layout



diamond

I20-2: Dispersive Branch



I20-2: Dispersive Branch

I20 hutches during construction phase

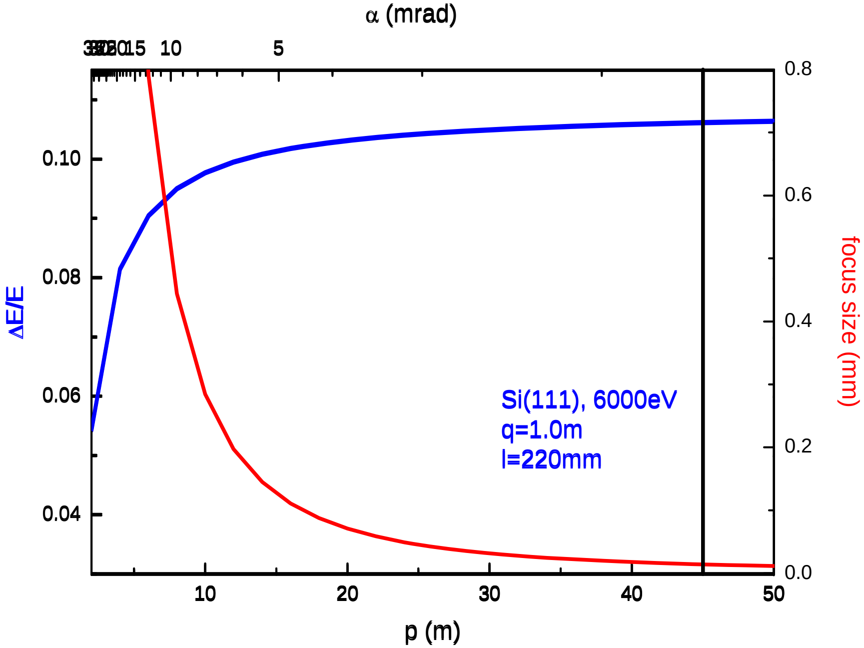
diamond

I20-2: Dispersive Branch

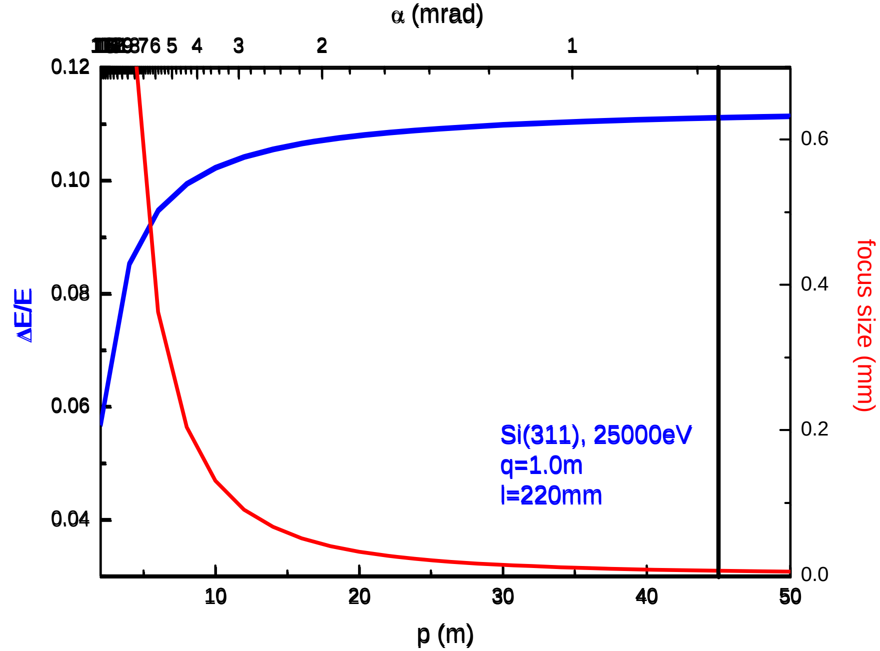
Two main criteria give the boundary conditions for the beamline design:

(i) Large energy bandpass (>10% over energy range)

(ii) Generous space around the polychromator focus (distance crystal-focus 1m).



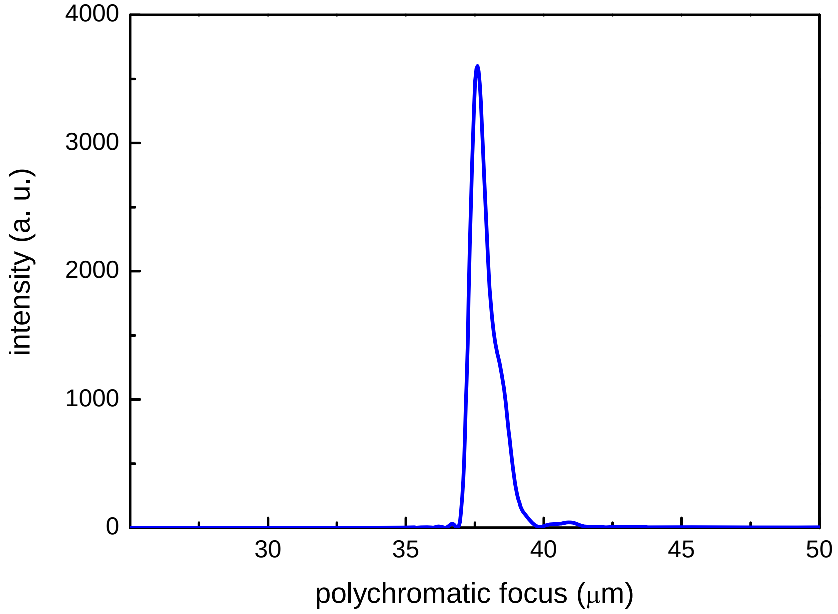
Si(111)



Si(311)

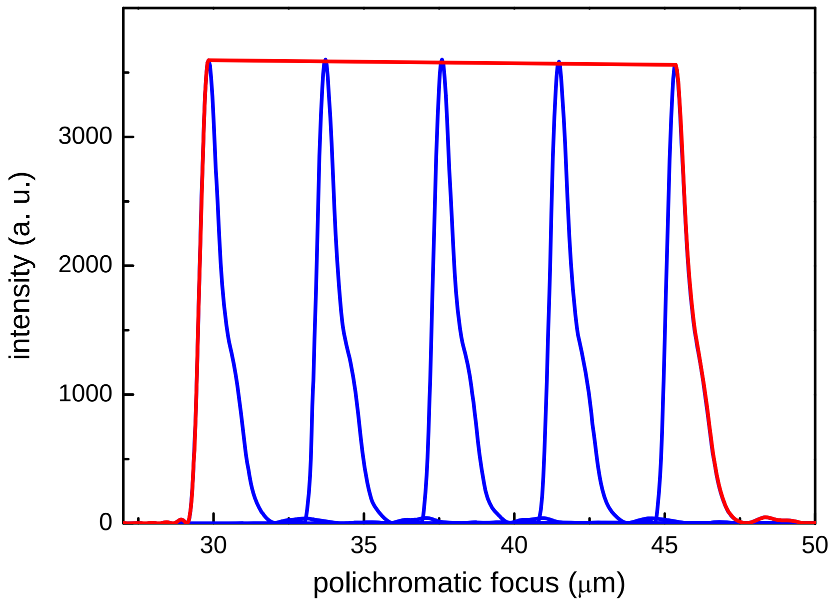
Using a horizontal aperture of 1.5mrad at 6keV will provide >10% bandpass by illuminating 220mm crystal length

I20-2: Dispersive Branch

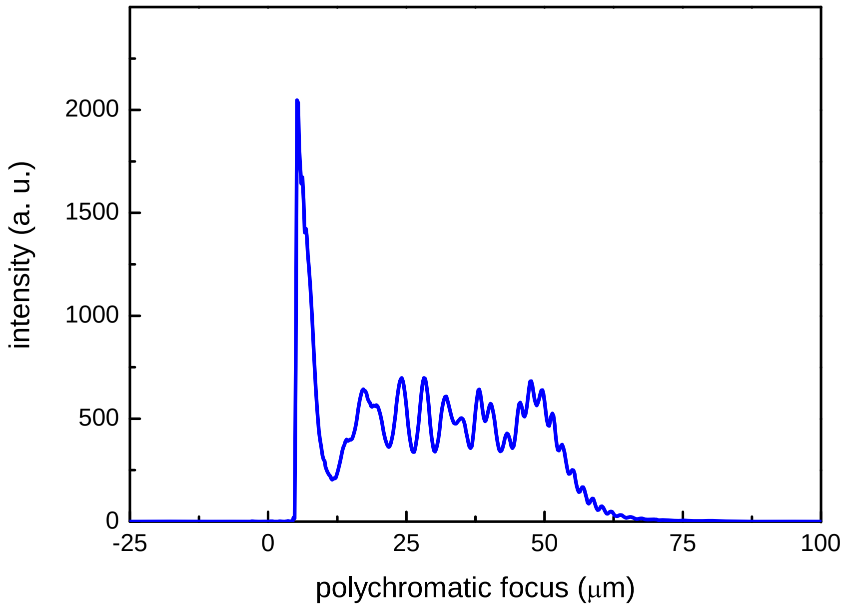


The full diffraction calculation shows a focus size of less than 5μm when considering a point source at 7keV.

If the finite size of the wiggler source is considered, the focus size calculated is in very good agreement with the geometrical calculations.

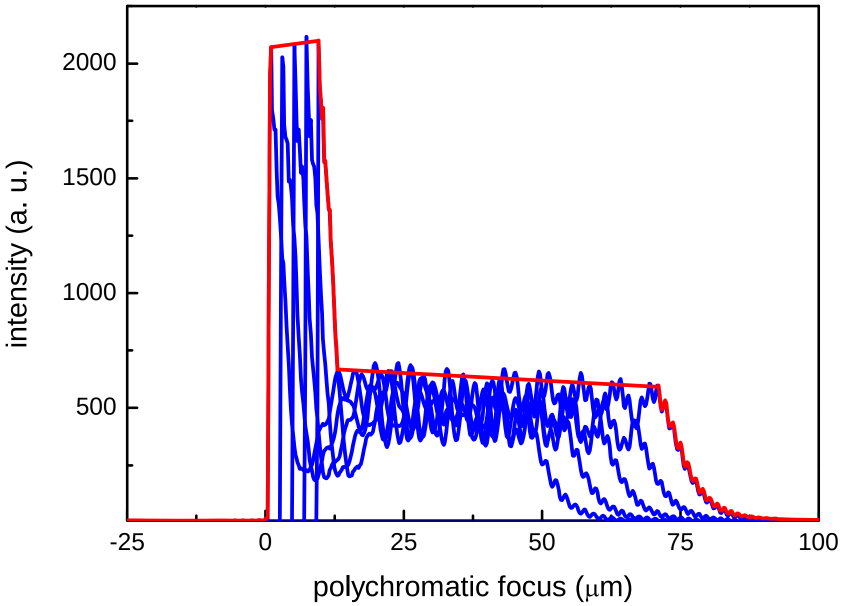


I20-2: Dispersive Branch



The same full treatment performed at 26keV using Si(311) give a focus size considerably larger than the geometrical calculations: the long tail appears due to the penetration of the x-rays.

As in the previous case, when considering the finite source size produced by the wiggler, the focus size increases.

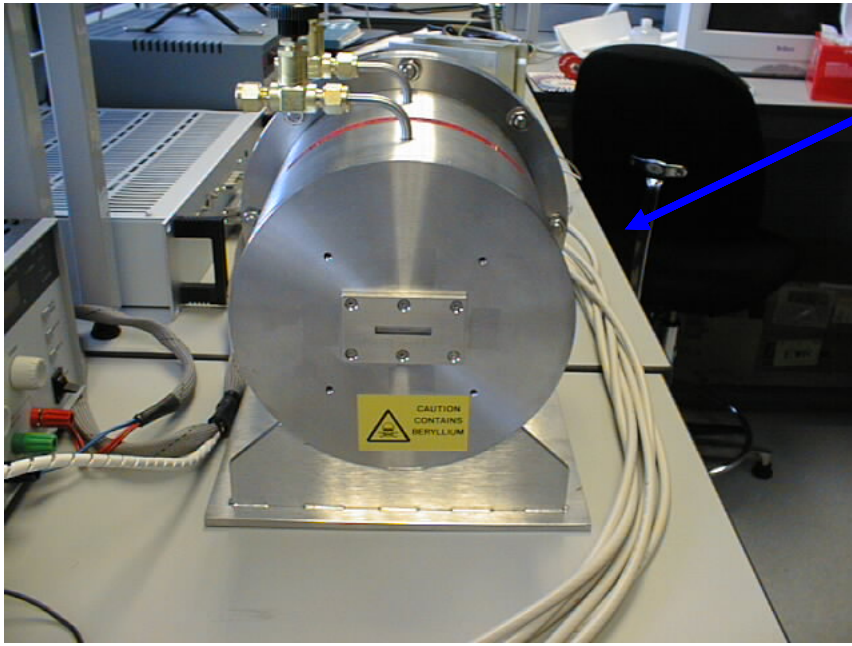


diamond

I20-2: Dispersive Branch
Optical elements

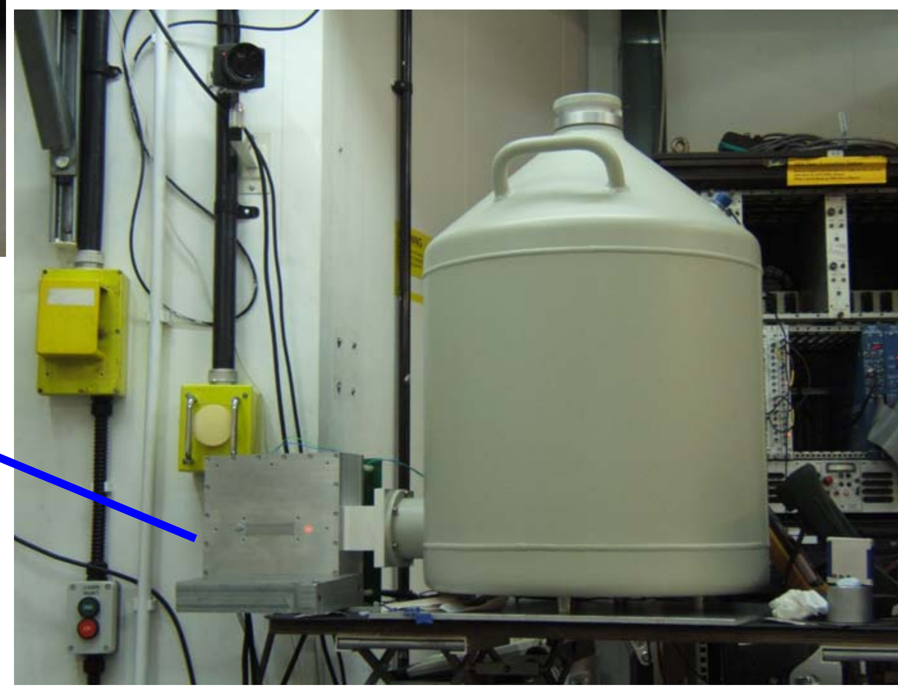
1. Vertical focussing mirror. Vertically deflecting flat mirror operating at 3mrad. Two different coatings will be used: platinum and rhodium.
2. Second mirror. Vertically deflecting flat mirror, operating at angles from 3mrad to 5mrad. Three different coatings will be used: bare silicon, rhodium and platinum.
3. Polychromator. Bragg configuration, Si(111) and Si(311). Future plans involve a Laue geometry polychromator with improved cooling.

Detectors



A silicon micro-strip detector will be used for the low energy operation. There are 1024 pixels, 25μm pitch.

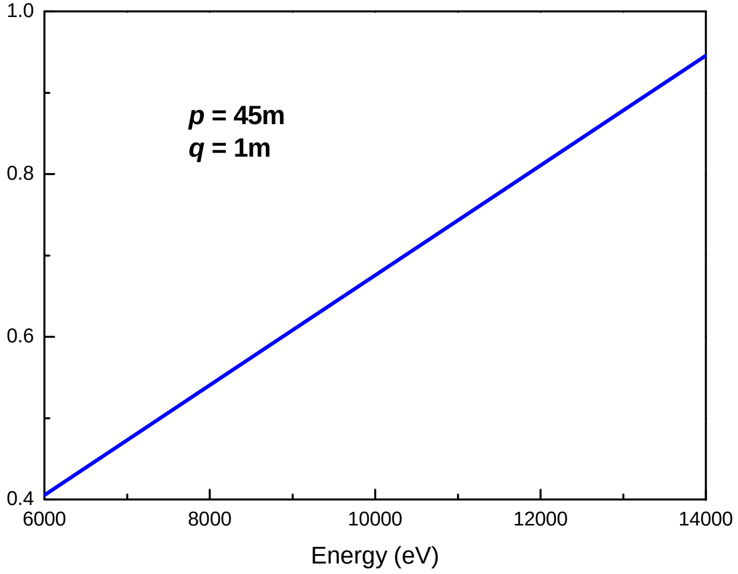
The minimum integration time is 1us, with 10μs readout time.



For high energies we will use a germanium micro-strip detector. There are 1024 pixels, 50μm pitch.

Detectors

Given the size of the detector, we should now calculate the distance at which it must be placed in order to collect the full fan of energies. As it is anticipated that different size horizontal apertures will be used for different energies, the detector position must be optimized.



Distance between the sample position and XSTRIP detector that is necessary to collect the full fan of energies as a function of energy.

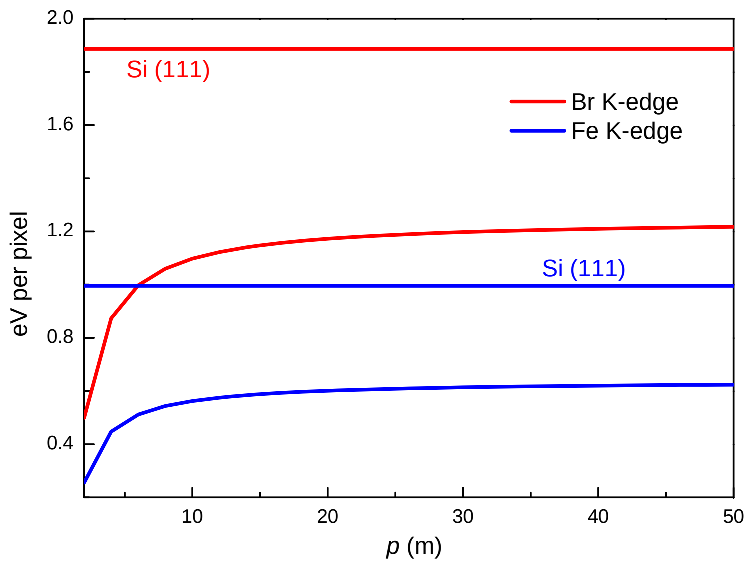
Note that at the lower energy (6keV) the distance is 0.4m.

What about the energy resolution?

Detectors

Three main factors affect the experimental energy resolution:

1. Crystal cut used in the polychromator : Si(111) or Si(311)
2. Pixel-size of the detector; distance sample-detector

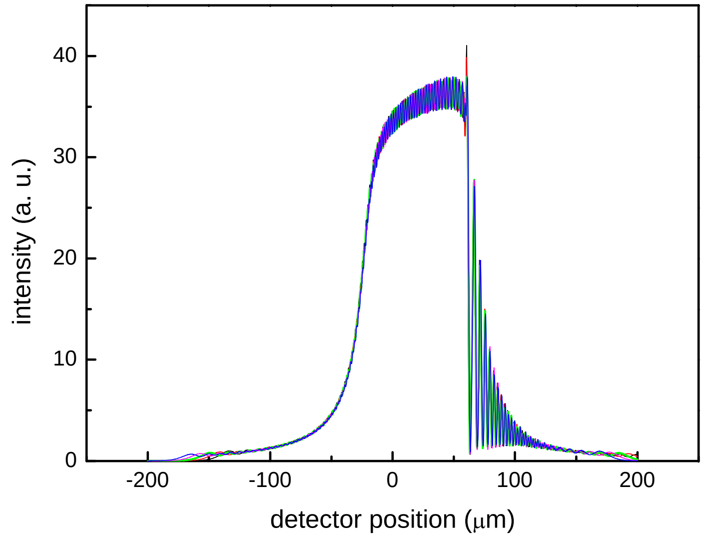


For the two extreme energies the resolution given by the detector is inside the intrinsic resolution of the Si(111)

Detectors

Three main factors affect the experimental energy resolution:

1. Crystal cut used in the polychromator : Si(111) or Si(311)
2. Pixel-size of the detector; distance sample-detector
3. Detector position: monochromatic focus



The focal distance for the 7000eV rays coming from the wiggler source is 2m from the polychromator crystal.

I20-2: Dispersive Branch

Main design characteristics for I20-2

(i) High flux
Choice of wiggler source

(ii) Large energy bandpass in order to achieve real EXAFS scans (>10% bandpass for all energy range).
Large divergence use

(iii) Generous space around polychromator focus for sample environment
'Large' distance between polychromator crystal and sample

(iv) Medium size focal spot

…and more important than all those:

No compromises for scanning XAS beamline, I20-1

I20

Team work:

Shusaku Hayama and Monica Amboage, Beamline scientists

John Sutter, Optics Scientist

Graham Duller, Mechanical Engineer

Mark Lunnon, Mechanical Technician

… and all the rest of support groups at diamond!!!