Summary of Beam Parameters and Other Requirements for LVPs at PETRA IV

Satellite workshop presentation

05-11-2020

DESY November meeting 2020

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LVP beamline mission(s)

Applications in geo- and material sciences:

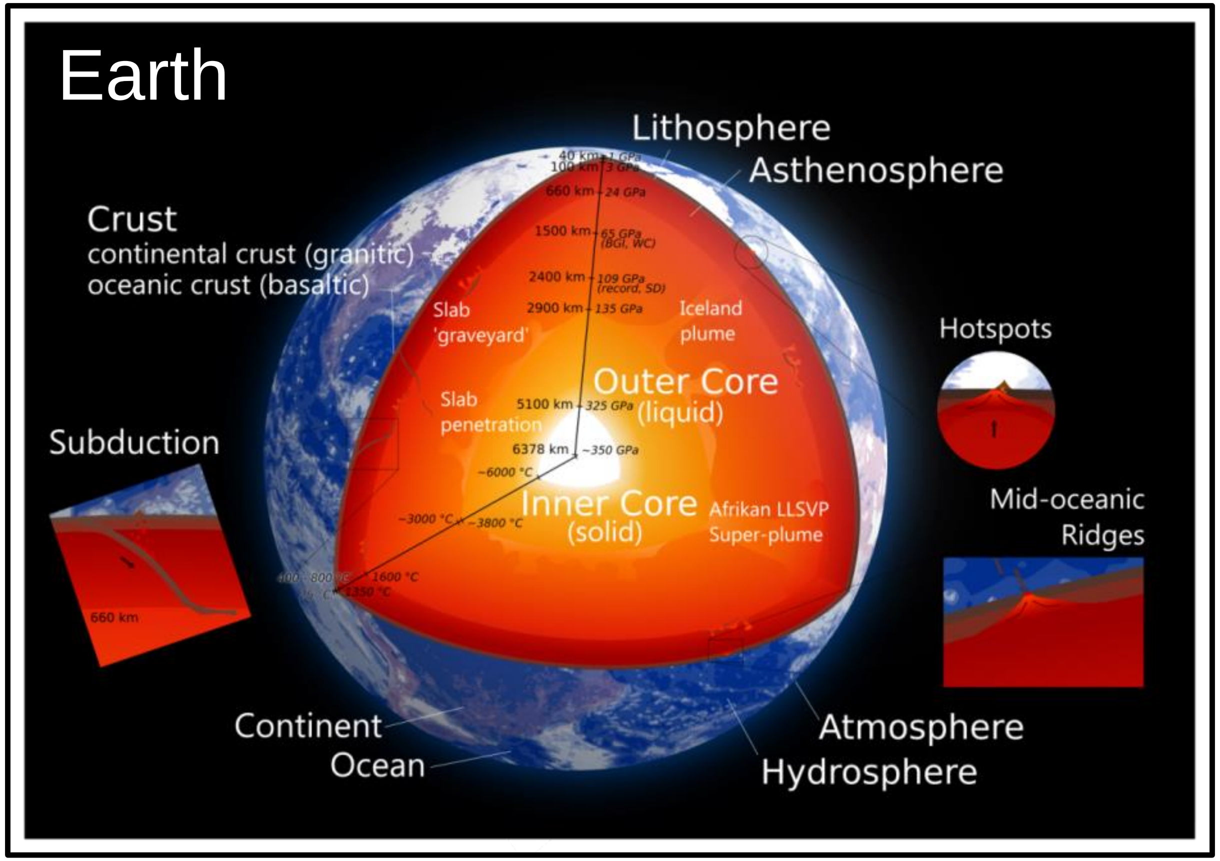
- Phase relations:
  - Transformation/nucleation
  - Melting curves (solidus/liquidus)
  - Equations of state
- Crystallography (w/ CAESAR or mono)
- Controlled rock deformation
- Melt viscosity measurements
- Structure of amorphous materials

Complementary *in situ* techniques:

- Ultrasonic interferometry
- Acoustic Emissions testing
- Electrical conductivity

Synthesis of novel functional materials

- Production feasibility (industry?)



P61B

- Ultra-high pressures (60±0.1 GPa)
- Large (100 mm^3) samples
- Polymineralic rock
  → Study of grain boundary transport properties (conduction, diffusion, rheology)

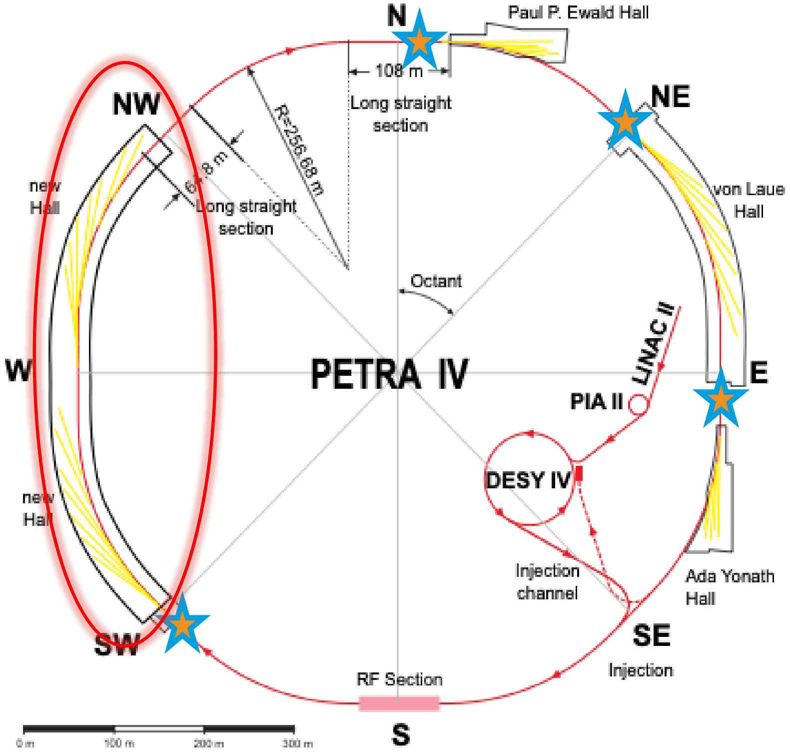
Outlook of PETRA IV.

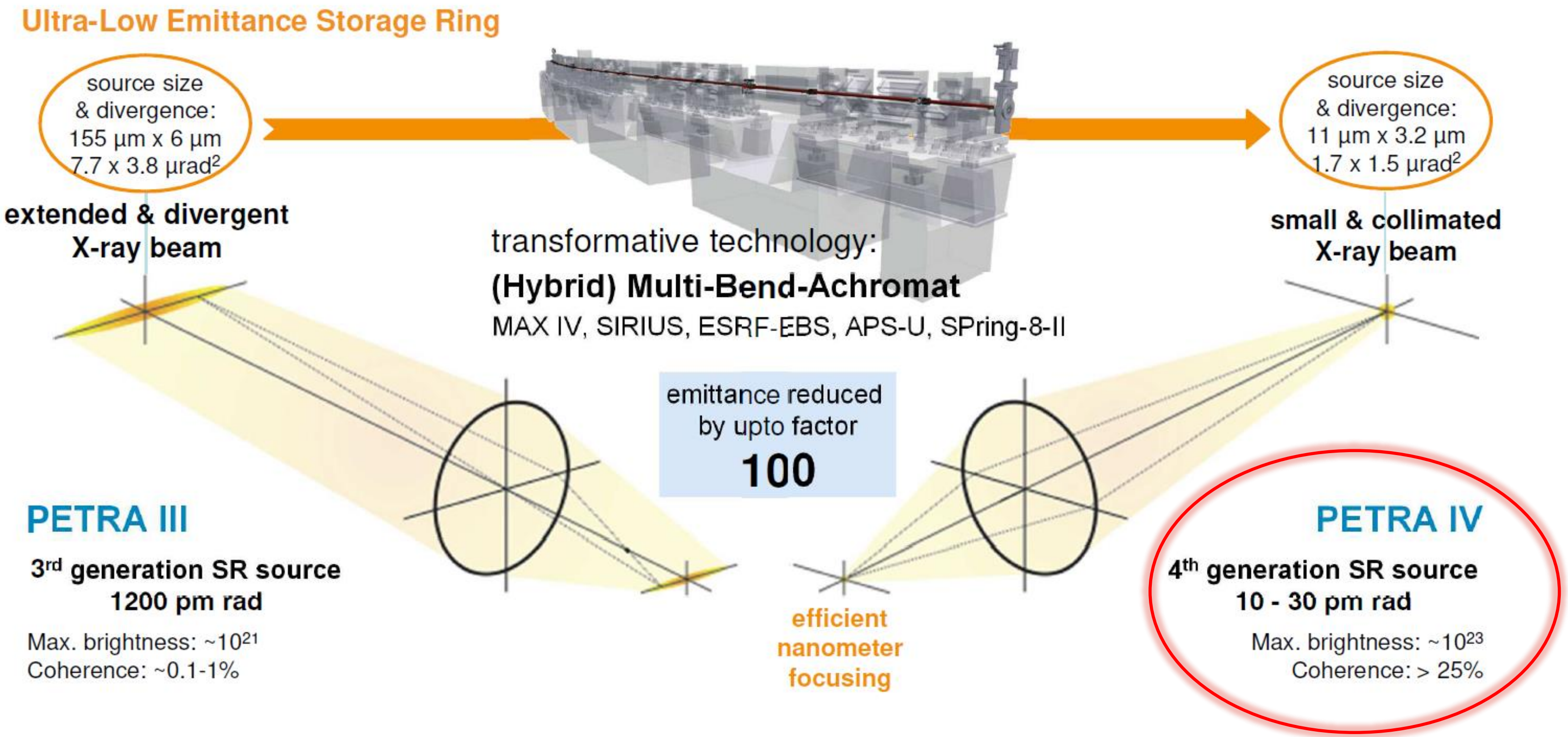
Conceptual Design of Storage Ring and Accelerator Complex

Design lattice:
Hybrid 7 Bend Achromat (H7BA)
adopted from ESRF-EBS

> **On-Axis Injection** using fast kickers

> Optimized **insertion devices** in long straight sections



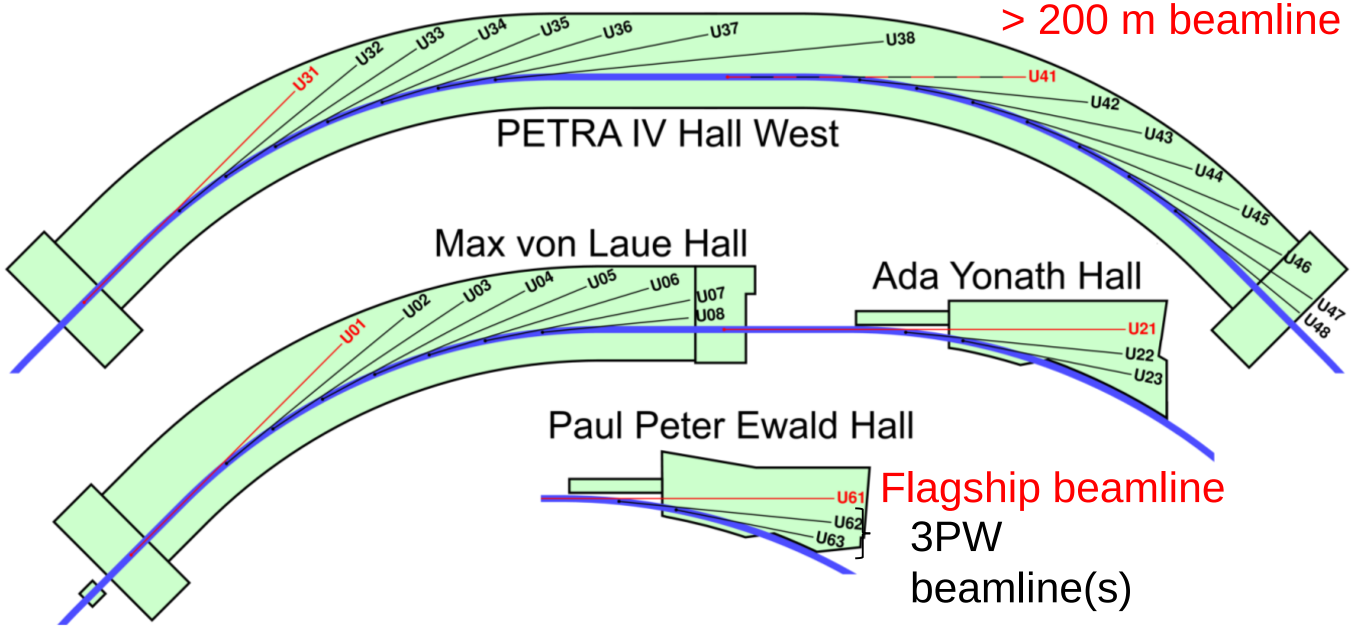


Beamlines at PETRA IV

…and the LVP beamline

More beamlines can be accommodated at P IV, than at PIII

- **PETRA IV takes 2 years to build**
  - Phase 1 beamlines (at launch) will be politically decided, incl. flagship beamlines.
  - Phase 2 beamlines (+1 yrs)
  - Phase 3 beamlines (+2 yrs?), the remainder.
- **‘Flagship beamlines’ dedicated to coherence methods or experiments requiring exceptional brilliance/timing**
  - Coherent Bragg-Diffraction Imaging (CDI)
  - Ptychography
  - Bunch Timing with high flux
- **BM/superbend in P. P. Ewald hall**
  Much less flux than now at P61B, particularly at higher energies (> 50 keV)



Some key questions:

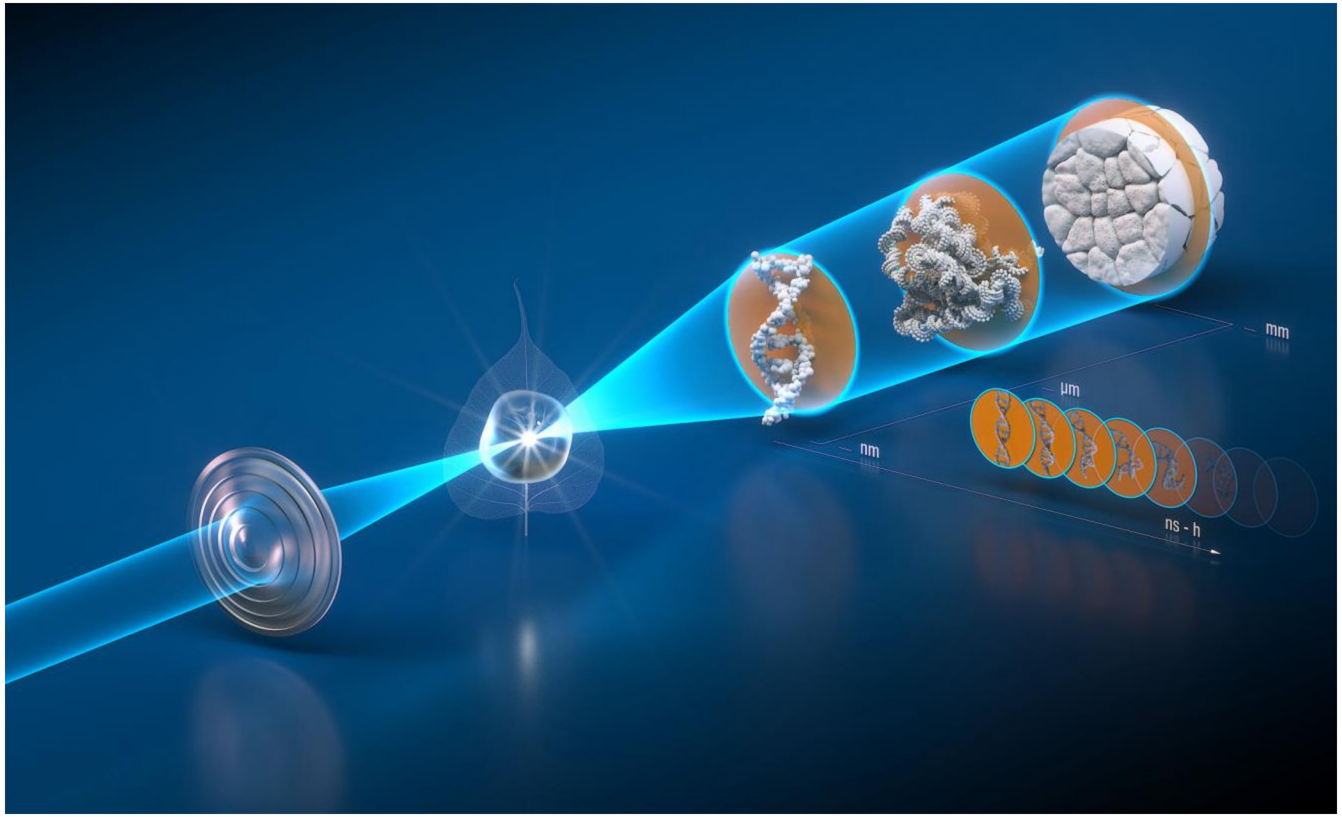
How long should the next LVP beamline be?

Should the new LVP beamline have more than 1 EH?

Calculations

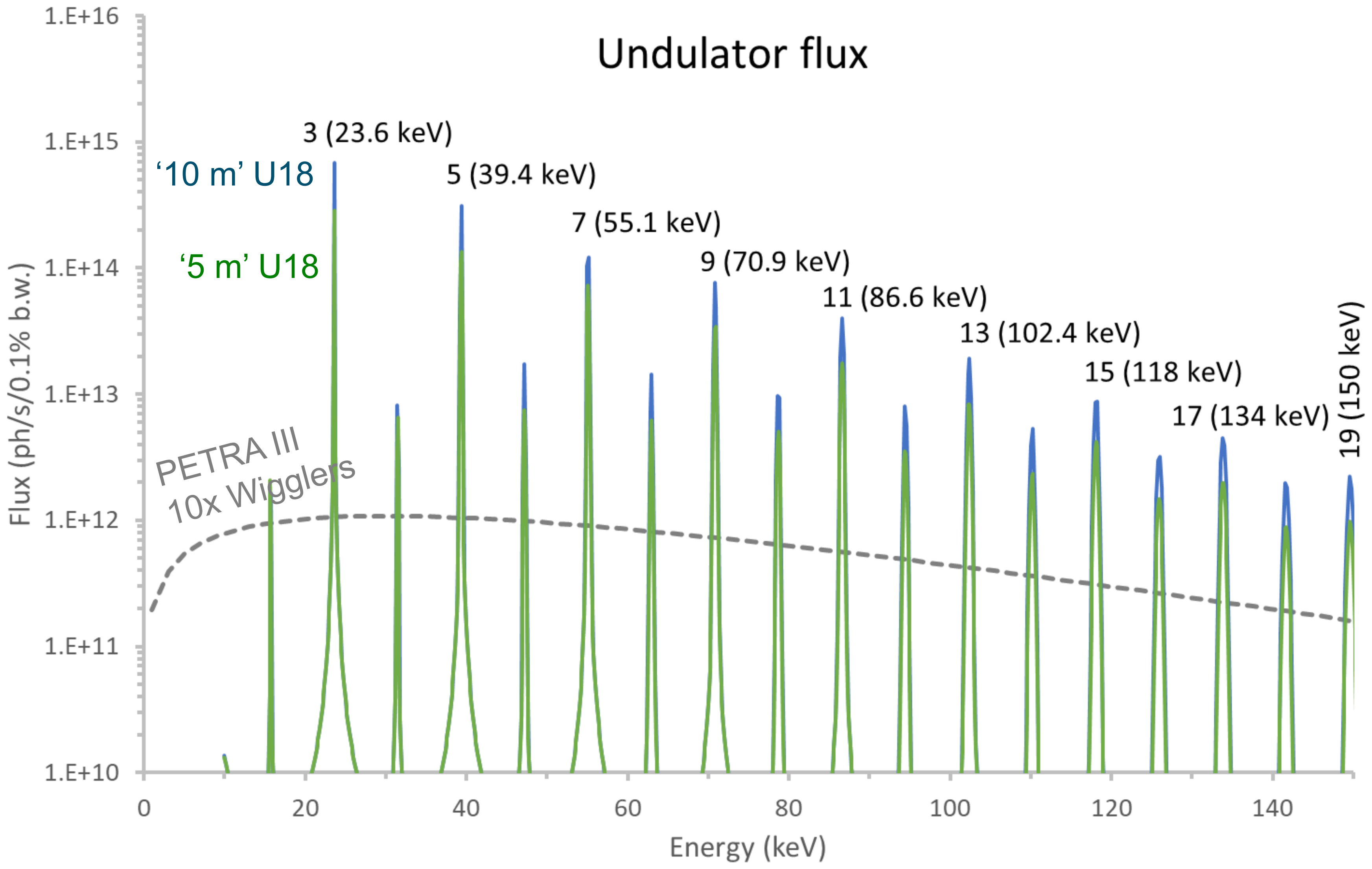
Overview

1. Photon flux
   - U18, 5m and 10m
   - Tuning curves
2. Beam size and distance
3. Expanding & focusing beams
4. Beam power



Photon flux – Brightness Mode

Calculations of photon flux at 150 m from the source in a 1 x 1 mm² aperture

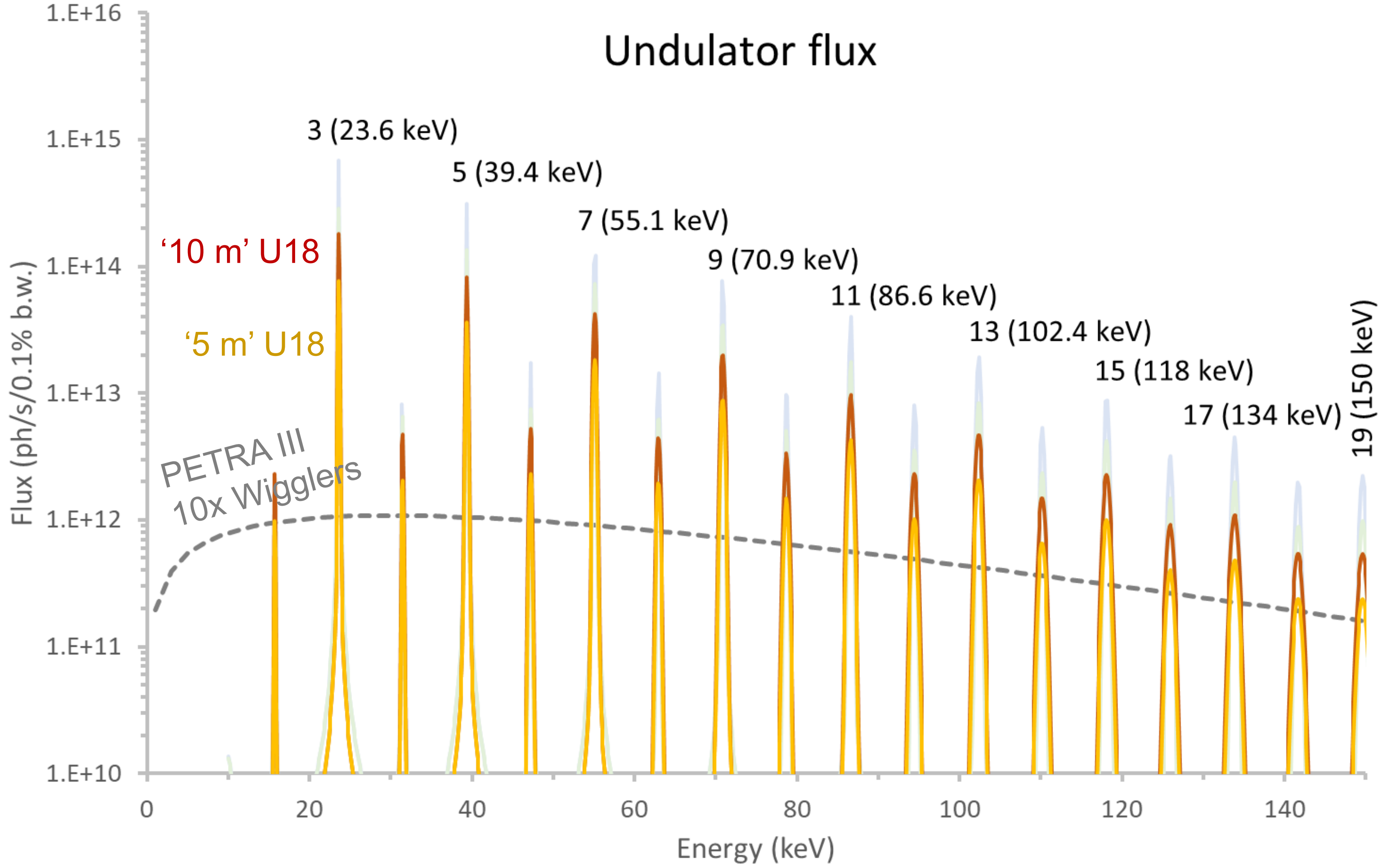


PETRA IV parameters:

- **Electron energy:**
  6 GeV
- **Average current:**
  200 mA (brightness),
  80 mA (timing)
- **Emittance:**
  < 20 pm rad (horz),
  < 4 pm rad (vert)
- **Number of bunches:**
  1600 (brightness),
  80 (timing)

Photon flux – Timing Mode

Calculations of photon flux at 150 m from the source in a 1 x 1 mm² aperture

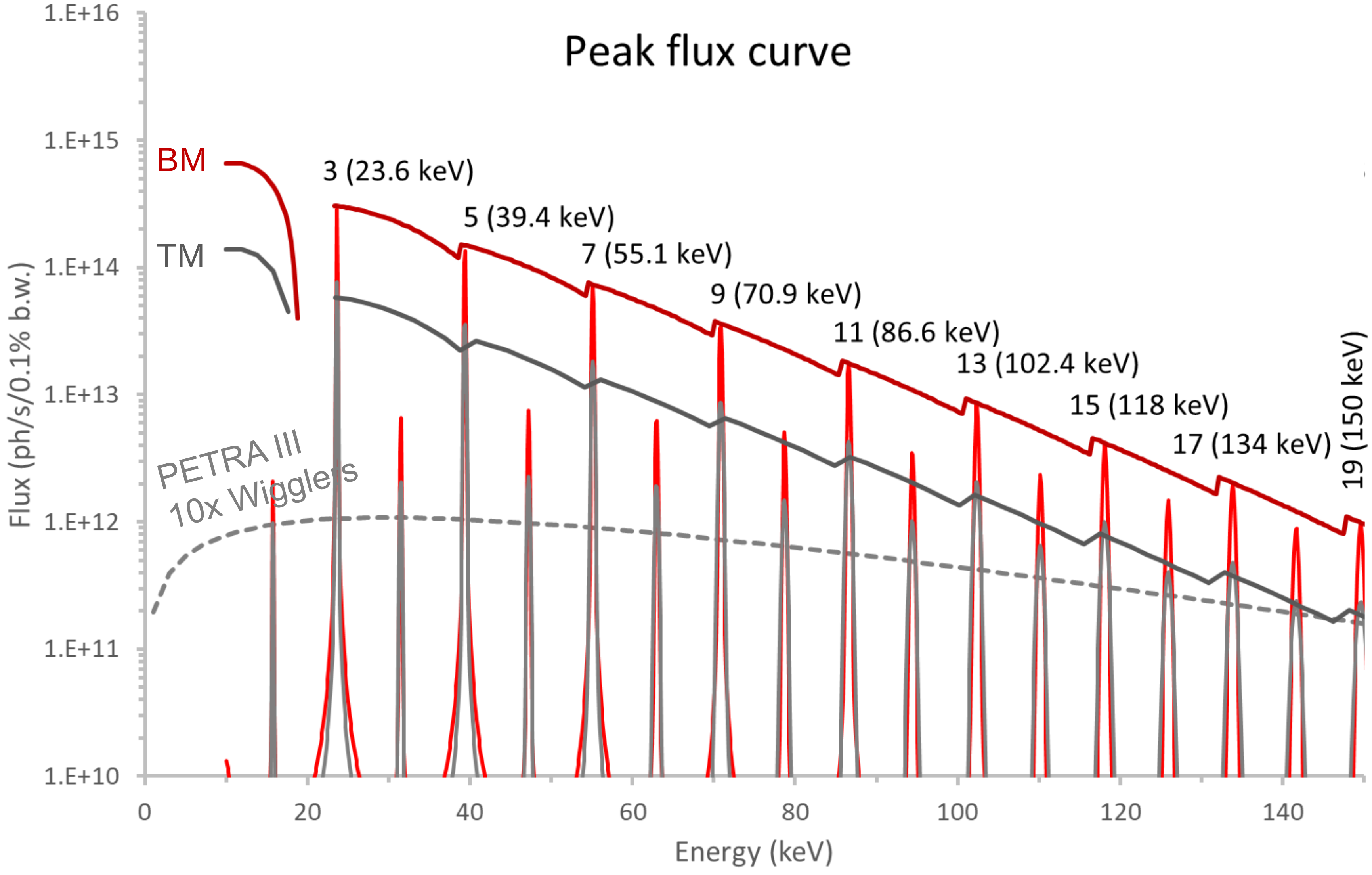


PETRA IV parameters:

- **Electron energy:**
  6 GeV
- **Average current:**
  200 mA (brightness),
  80 mA (timing)
- **Emittance:**
  < 50 pm rad (horz),
  < 10 pm rad (vert)
- **Number of bunches:**
  1600 (brightness),
  80 (timing)

Photon flux – '5 m' undulator U18

Calculations of photon flux at 150 m from the source in a 1 x 1 mm^2 aperture



PETRA IV

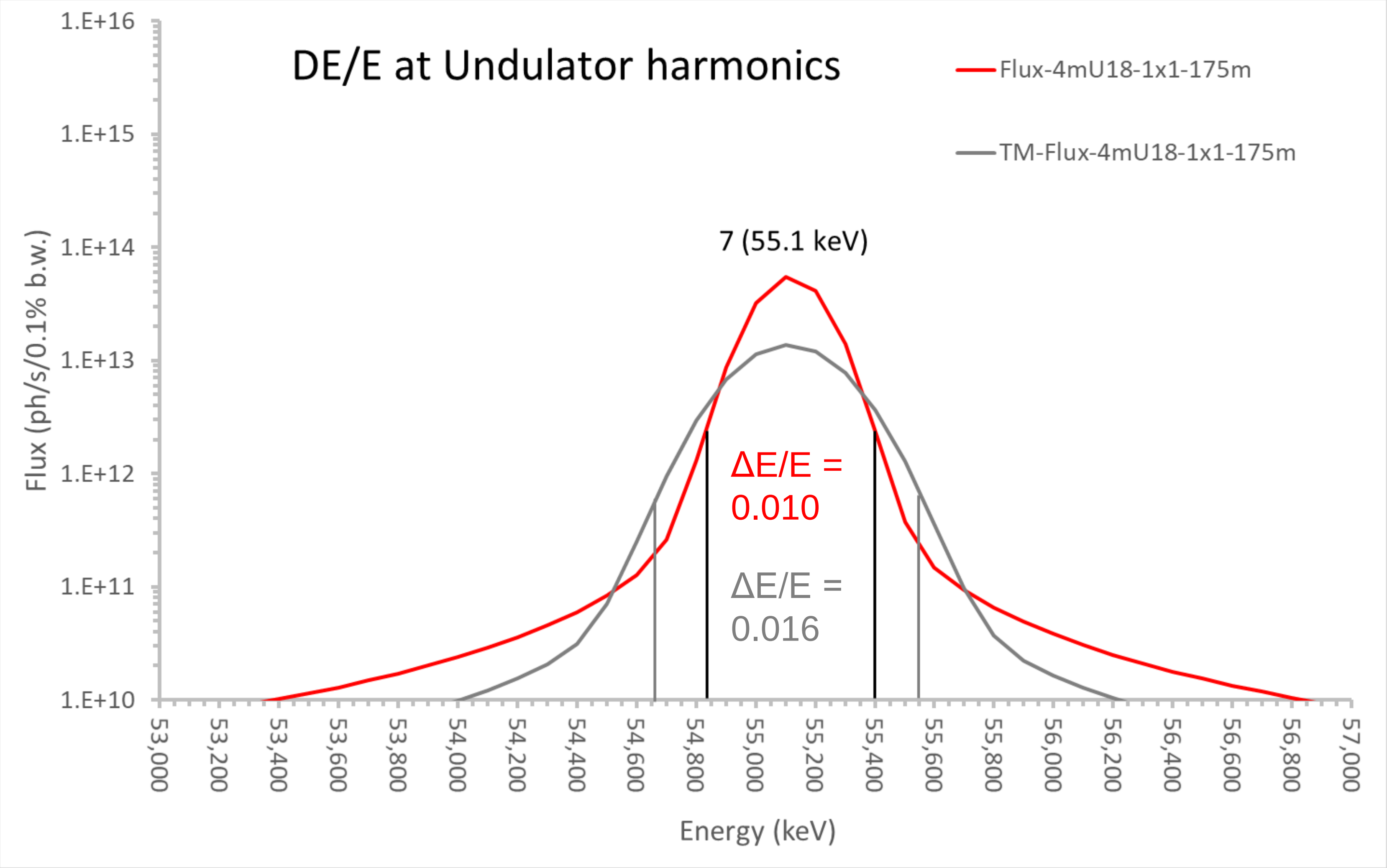
- Brightness Mode (200 mA – 1600 bunch)
- Timing Mode (80 mA – 80 bunch).

- By tuning the undulator strength parameter, *K* the peak flux curve is obtained for each harmonic.

Note: This parameter can only be one value at a time, hence not all of this radiation is available at the same time!

IV. Beam characteristics for the instruments (LVP)

Energy resolution on a harmonic (‘pink beam’)

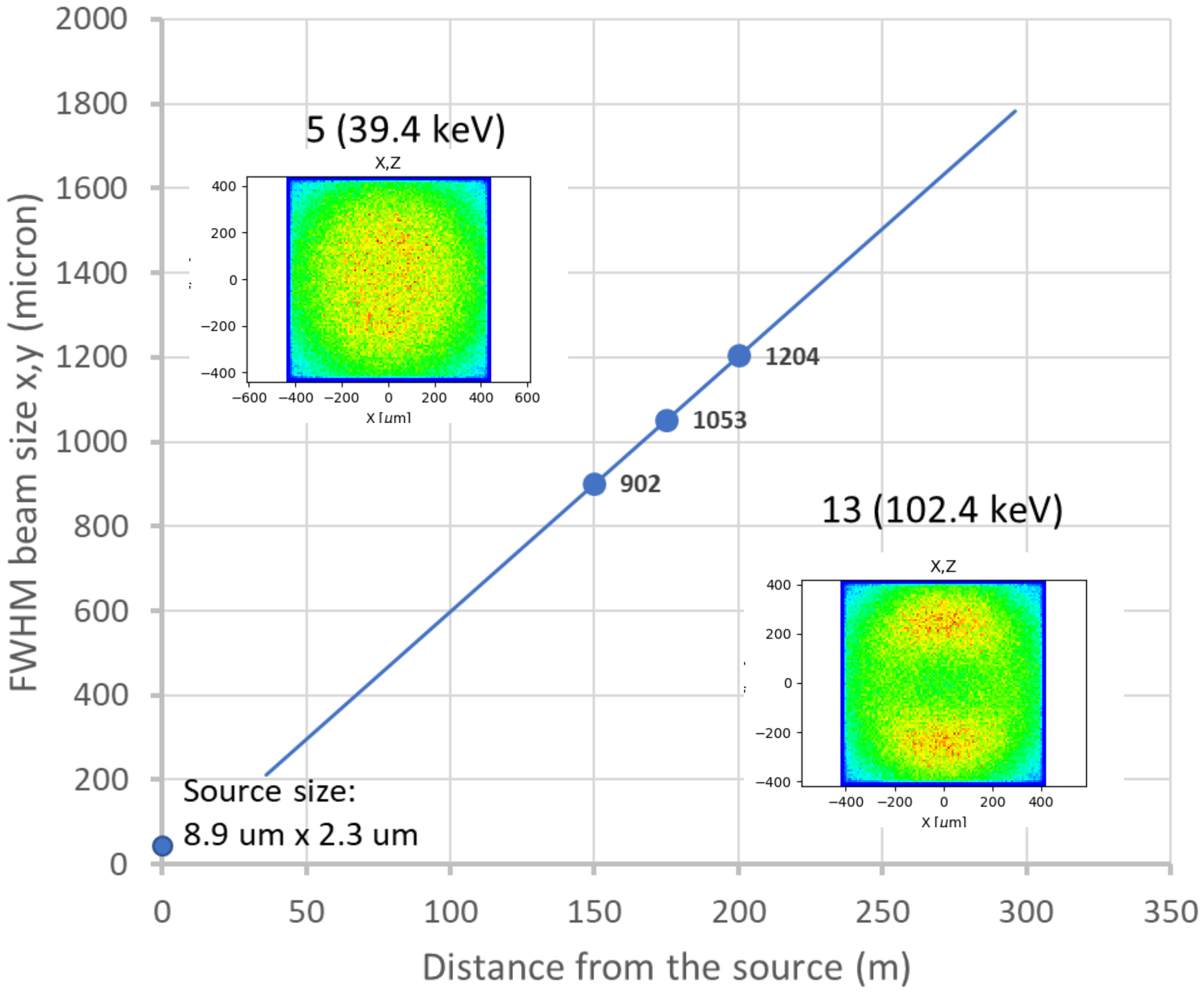


The energy resolution on a harmonic may not be quite as satisfactory (using ‘pink beam’ techniques).

Bent double-xl Laue monochromator, optimized for high throughput, will improve ΔE/E to ~10^{-3}

Beam size

Bigger is better? Problem of low divergence at PETRA IV



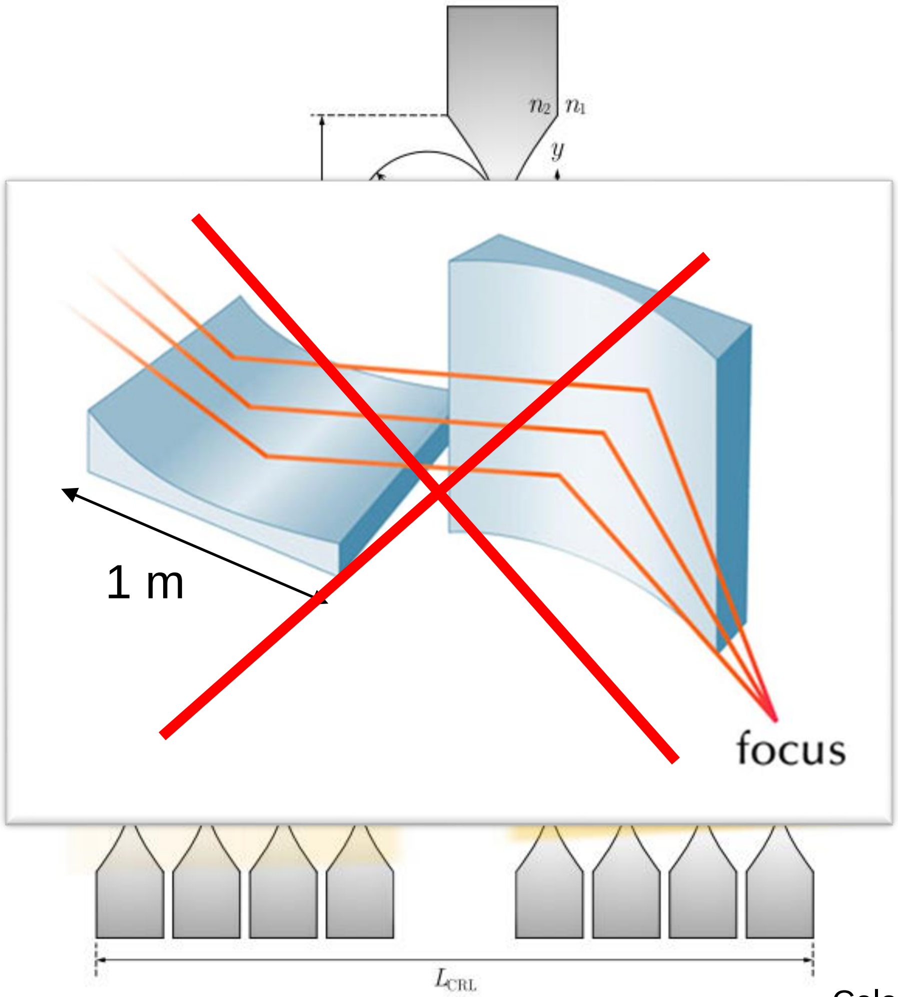
Due to the small source size and low divergence in the beam, *uniform beam size* is small even at large distances.

- Beam size is approx. 0.9 x 0.9 mm^2 at 150 m.
- Beam size is approx. 1.2 x 1.2 mm^2 at 200m.

Beam size needs to be expanded another way! (A few beamlines can be over > 200 m long at PETRA IV)

Beam size

Understanding Compound Refractive Lenses (CRLs)



(b) N-stacked lenses to form a CRL

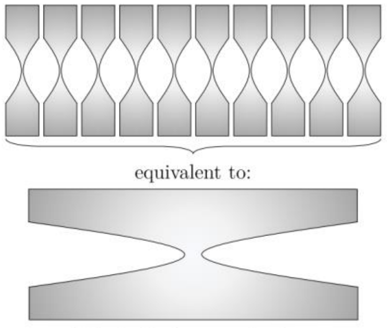
Celestre et al.
ESRF 2019

- Parabolic lenses are the most used X-ray lenses in CRL and always present a very good approximation to geometric focusing and reduce the geometrical aberrations.
- To overcome the weak refraction of a single element, several X-ray lenses are stacked. Focal distance:

$$f_{\text{thin CRL}} = \frac{R_{x,y}}{2N\delta},$$

- Aperture

$$A_{x,y} = 2\sqrt{(L - \text{t}_{\text{wall}})R_{x,y}},$$



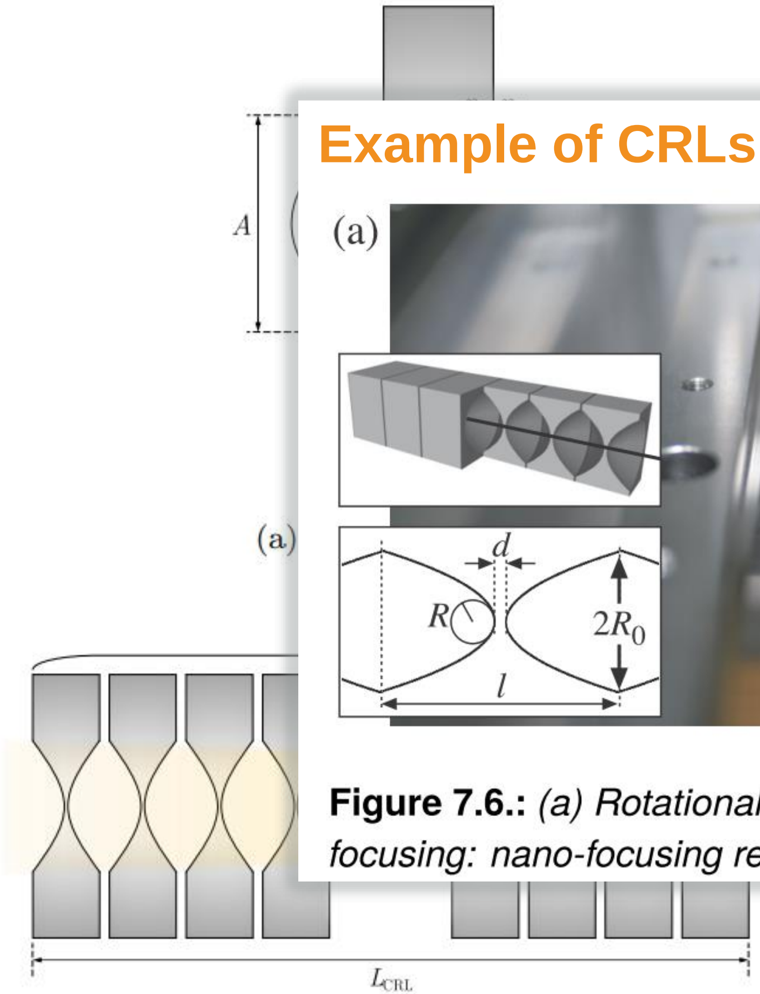
(a) single lens equivalent

E.g. if we want A_{xy} = 0.5 mm beam, and $R_{x,y}$ = 20 µm, lenslet thickness should be 3.1 mm each!

Beam size

Understanding Compound Refractive Lenses (CRLs)

- Parabolic lenses are the most used X-ray … a very … ocusing … tions. … f a single … stacked.



(b) N-stacked lenses to form a CRL

Example of CRLs for nano-focusing

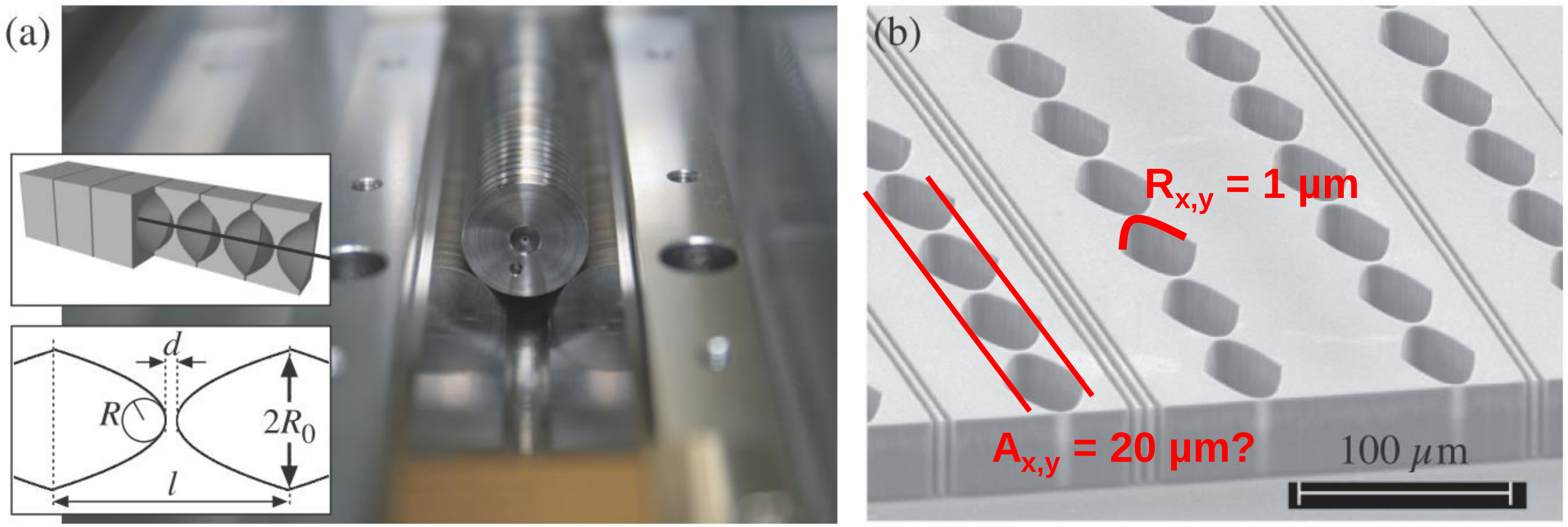
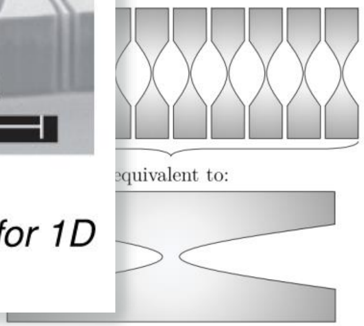


Figure 7.6.: *(a) Rotationally parabolic refractive X-ray lens. (b) Parabolic cylinder lenses for 1D focusing: nano-focusing refractive X-ray lenses (NFLs) made of silicon.*

$$A_{x,y} = 2\sqrt{(L - t_{wall})R_{x,y}},$$

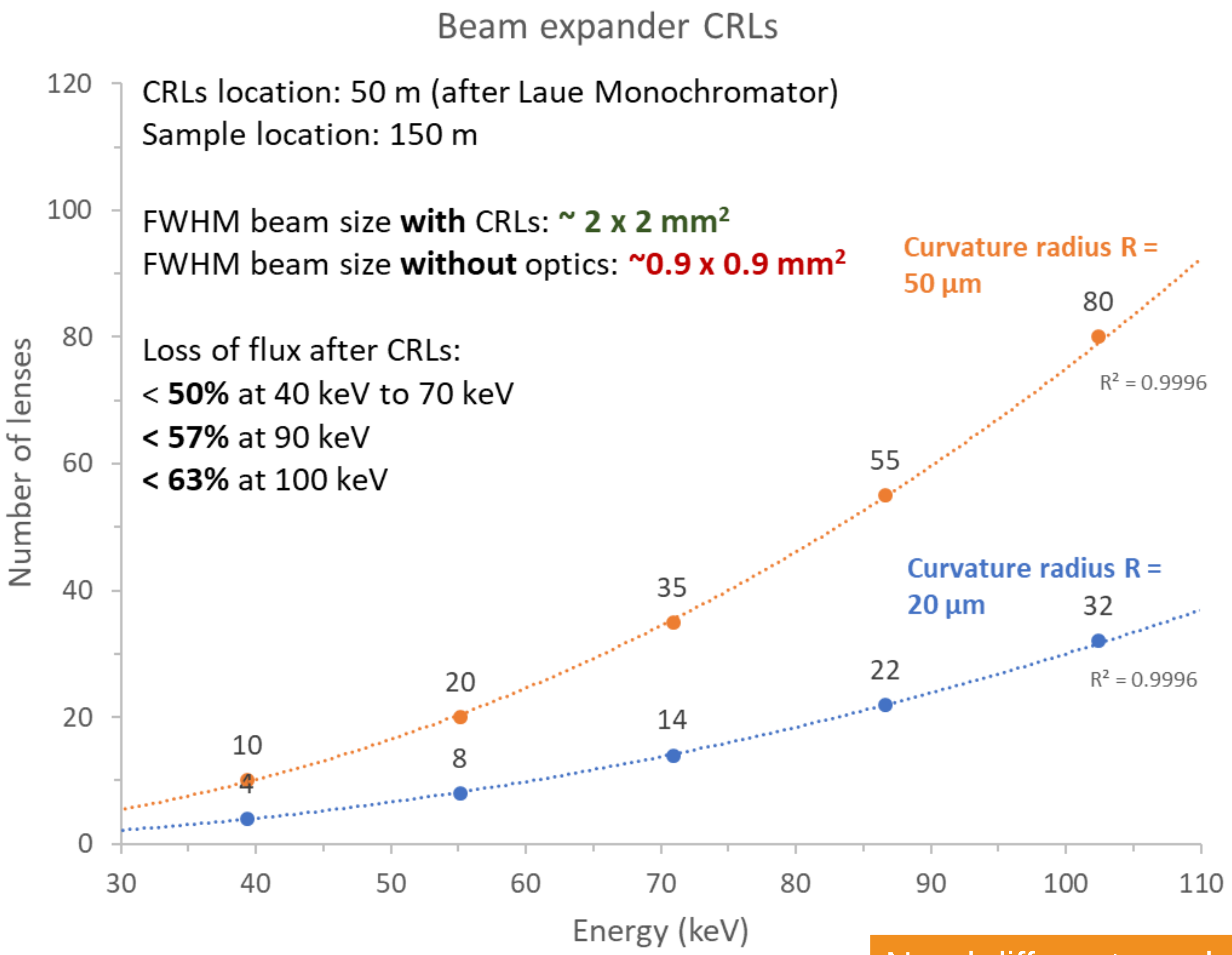


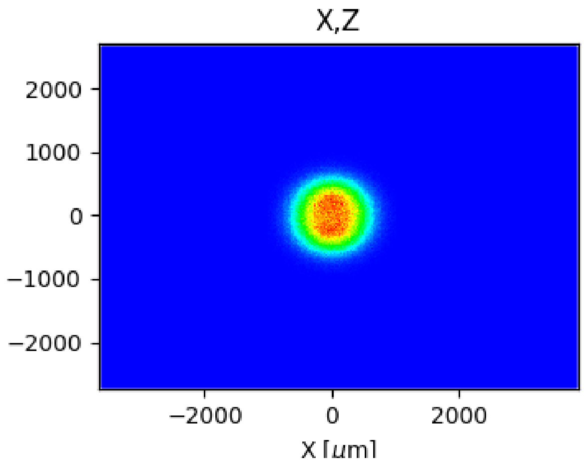
(a) single lens equivalent

Celestre et al.
ESRF 2019

Beam size

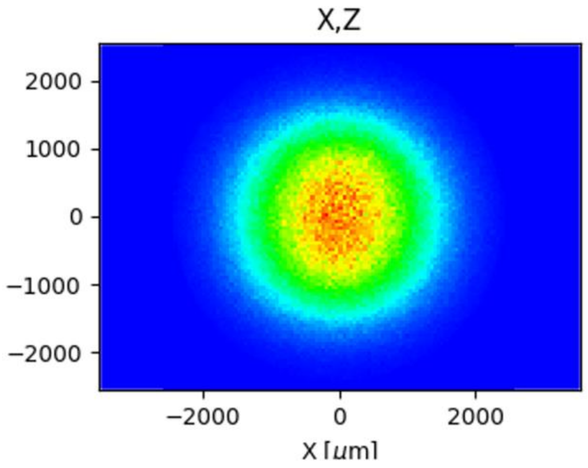
Expanding beam using Si Compound Refractive Lenses (CRLs) for imaging





Normal beam size @ 150 m

0.9 x 0.9 mm^2 FWHM



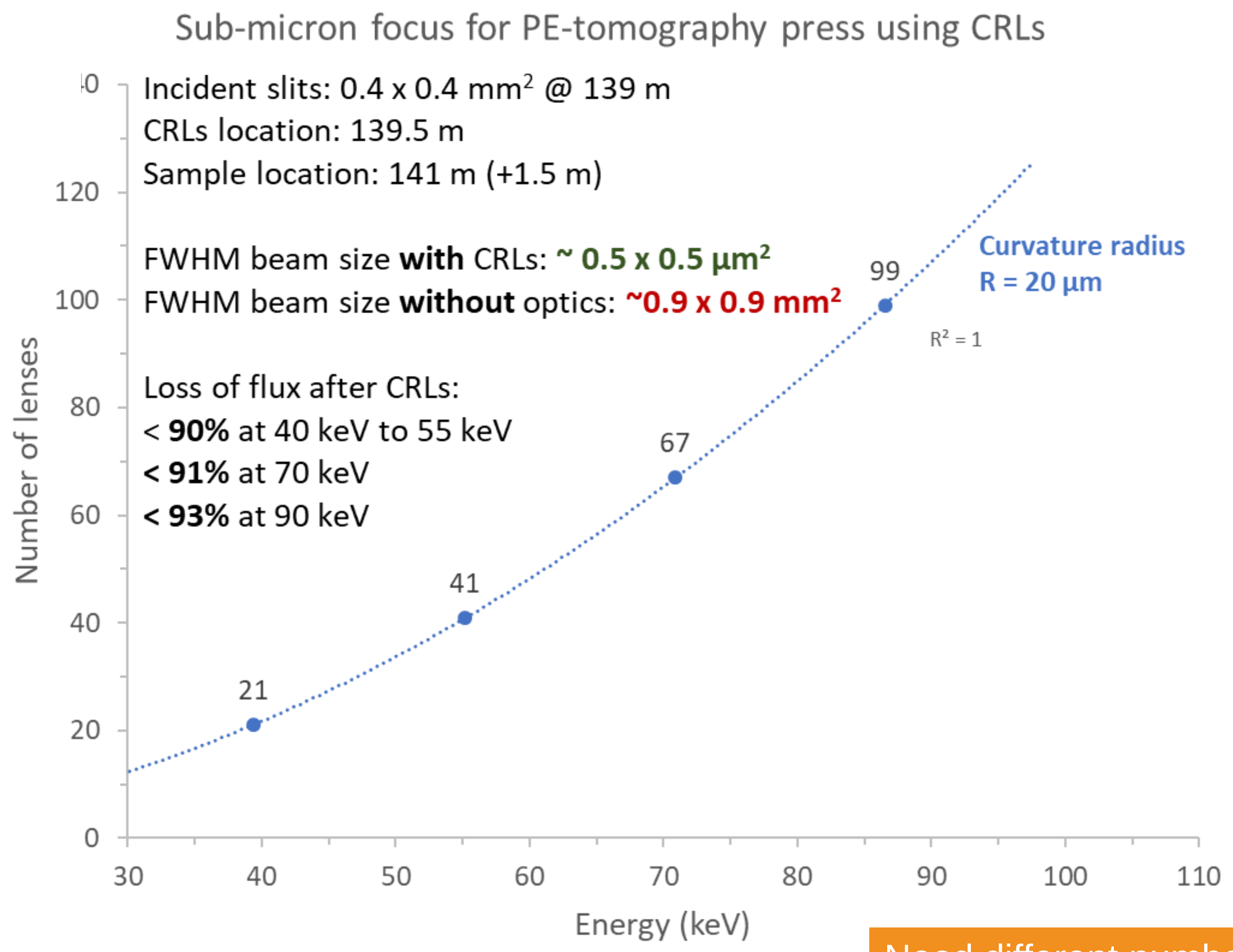
Expanded beam size @ 150 m

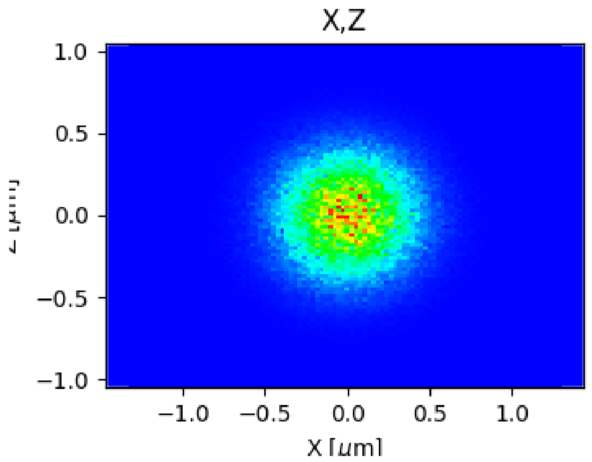
> 2 x 2 mm^2 FWHM

Need different number of CRLs for each energy!

Beam size

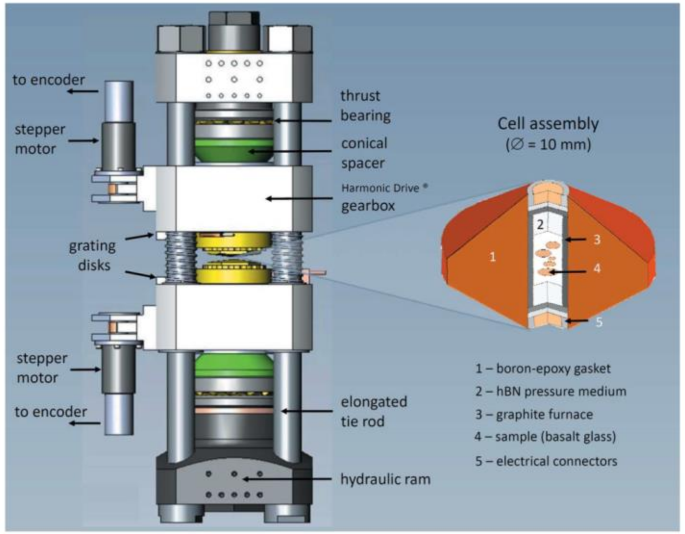
Focusing beam using Si Compound Refractive Lenses (CRLs) for XRD, or X-ray tomography





Focused beam size
@ 150 m

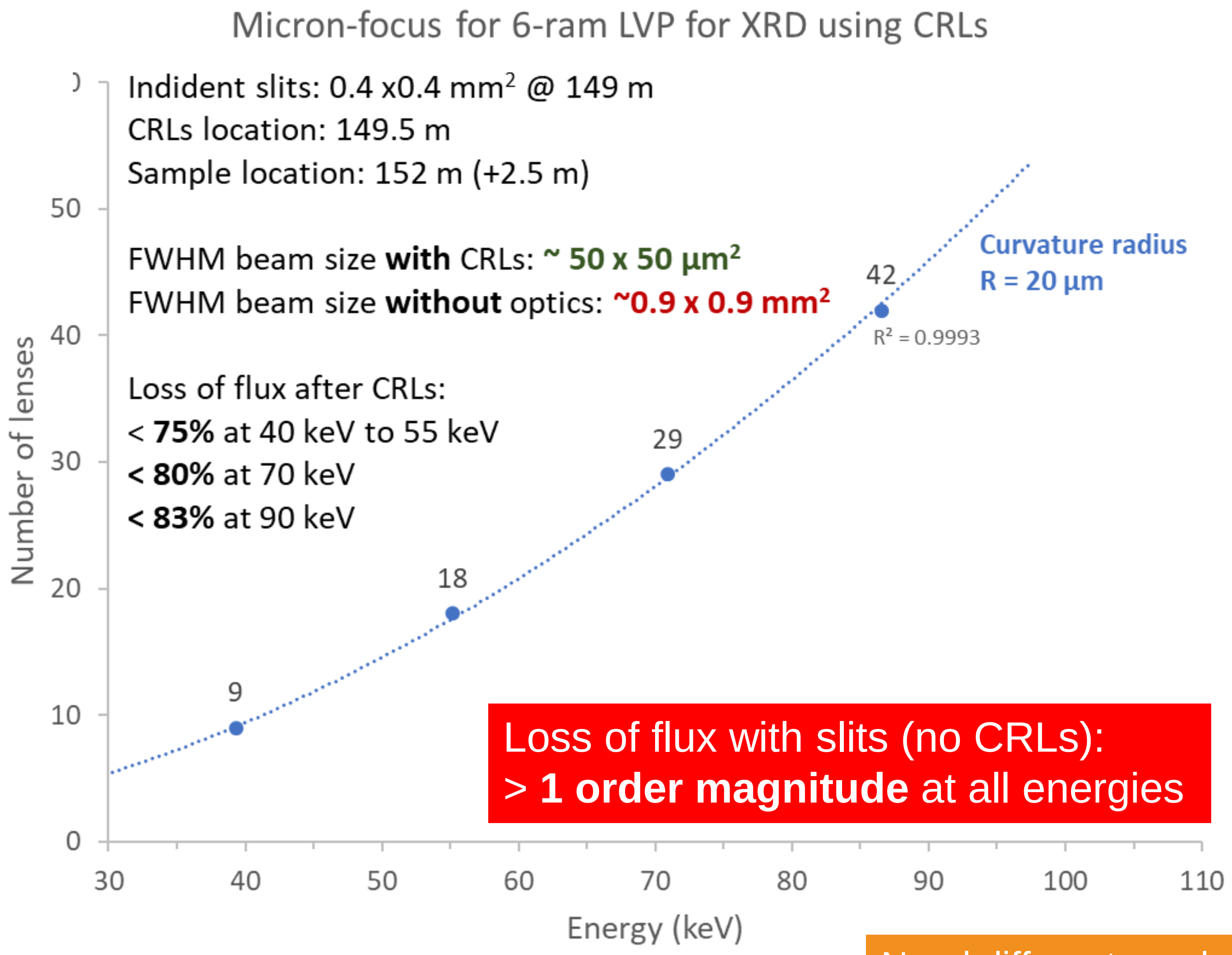
< 0.5 x 0.5 µm²
FWHM



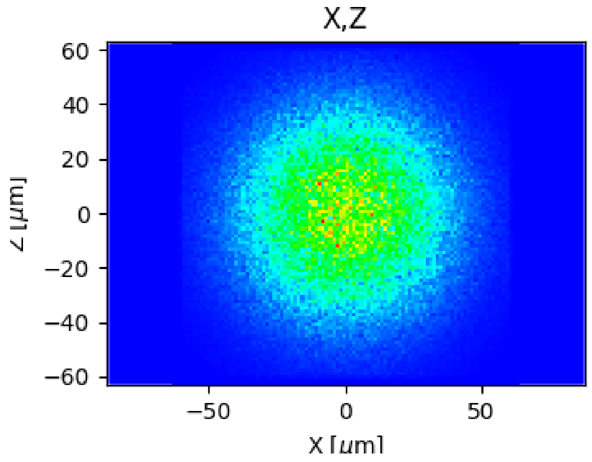
Need different number of CRLs for each energy!

Beam size

Focusing beam using Si Compound Refractive Lenses (CRLs) for XRD, or X-ray tomography

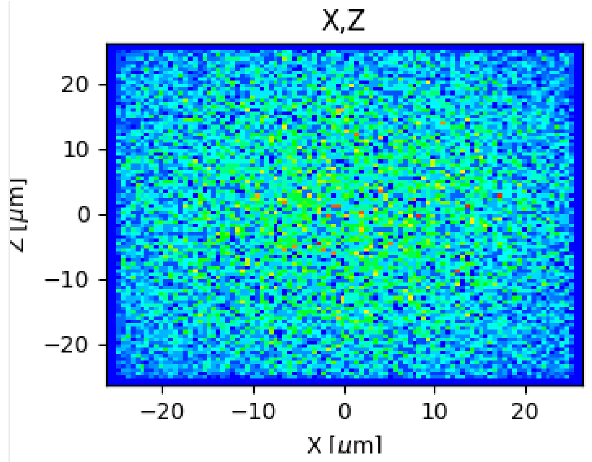


Loss of flux with slits (no CRLs):
> **1 order magnitude** at all energies



Focused beam size
@ 150 m

e.g.
50 x 50 µm²
FWHM

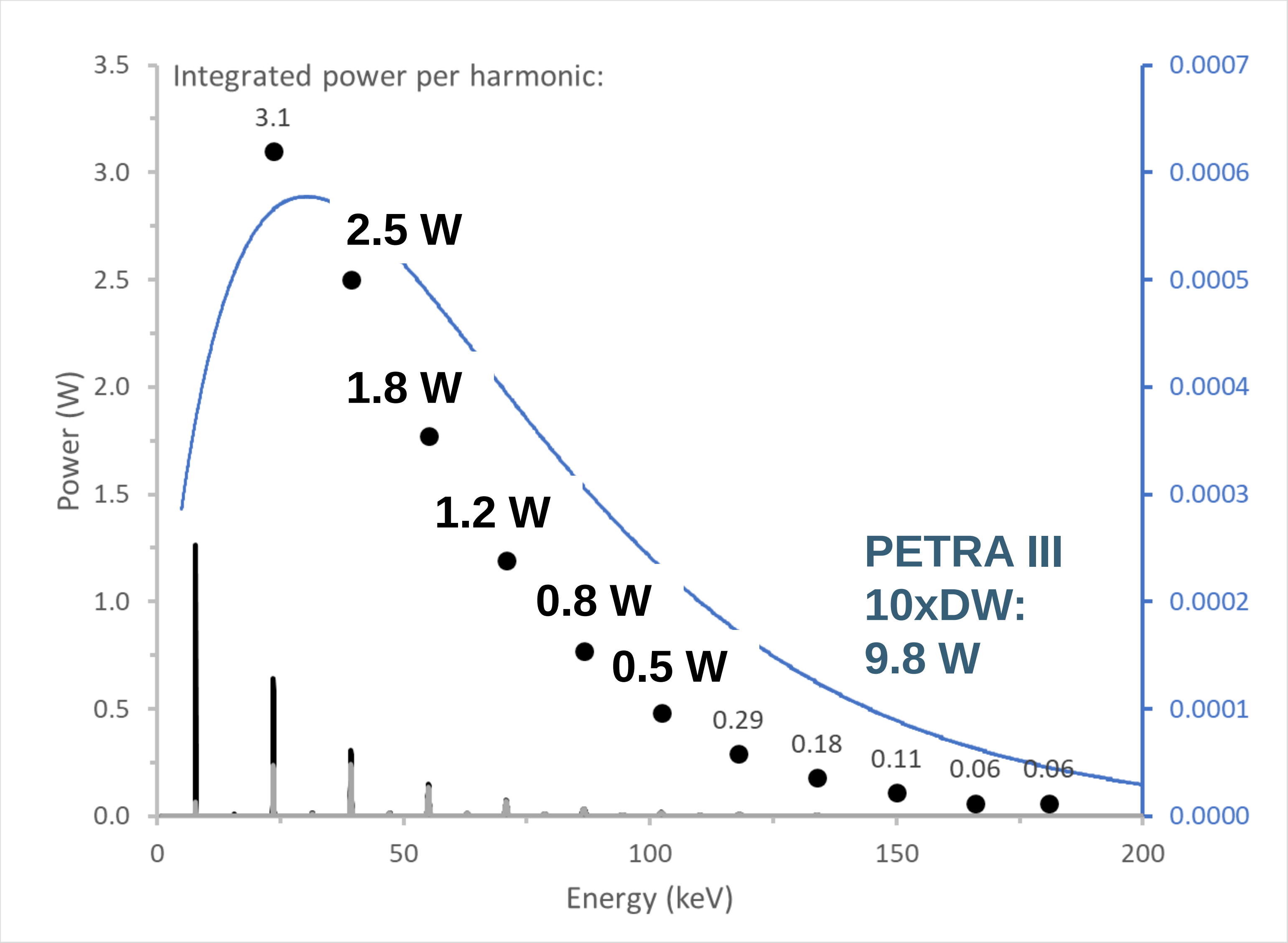


Slits after CRLs
50 x 50 µm²
aperture

Need different number of CRLs for each energy!

Power

Calculations of undulator power at beamline U61 (136 m from the source)



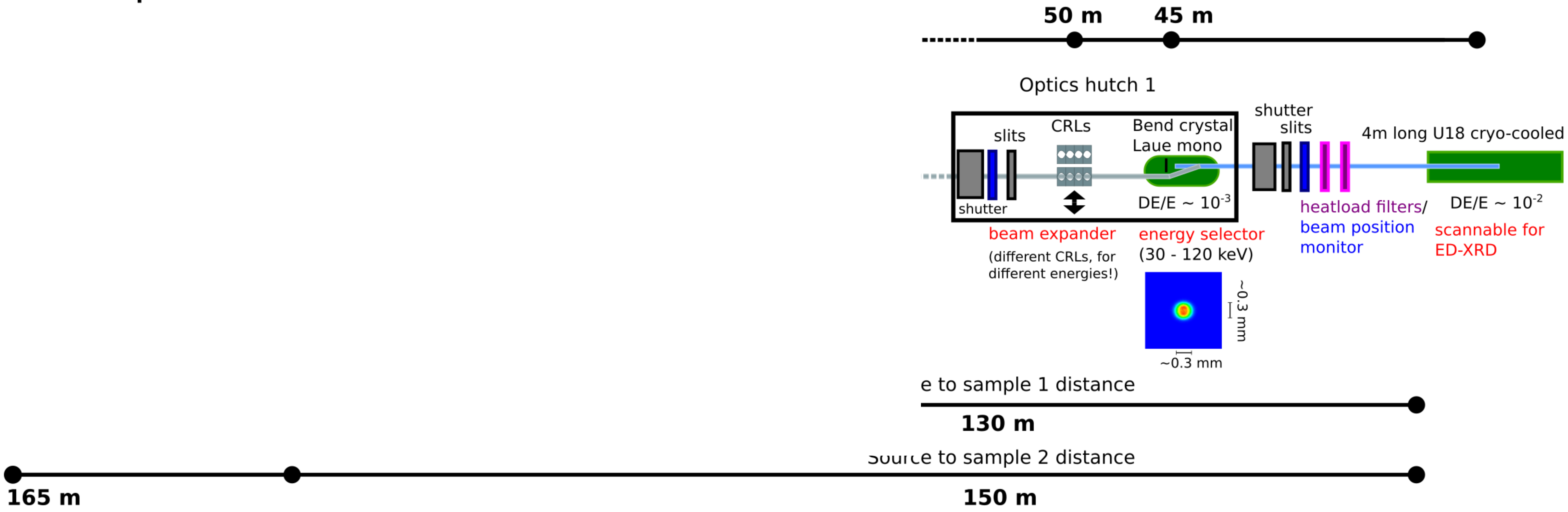
Power density for all harmonics at a distance > 136 m

Considering low keV heat load filters, a monochromator, CRLs, the high-flux monochromatic beam very low power.

Little chance of heating the sample with a high flux beam at PETRA IV.

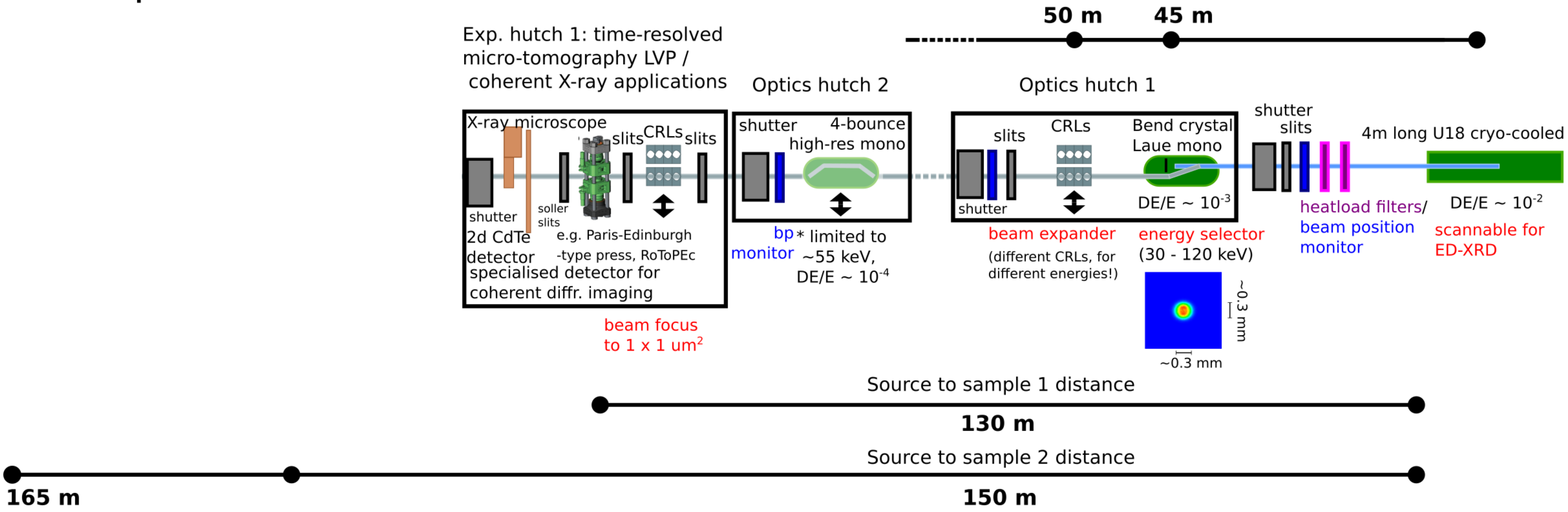
Example PETRA IV beamline for LVPs

Concept LVP beamline for PETRA IV

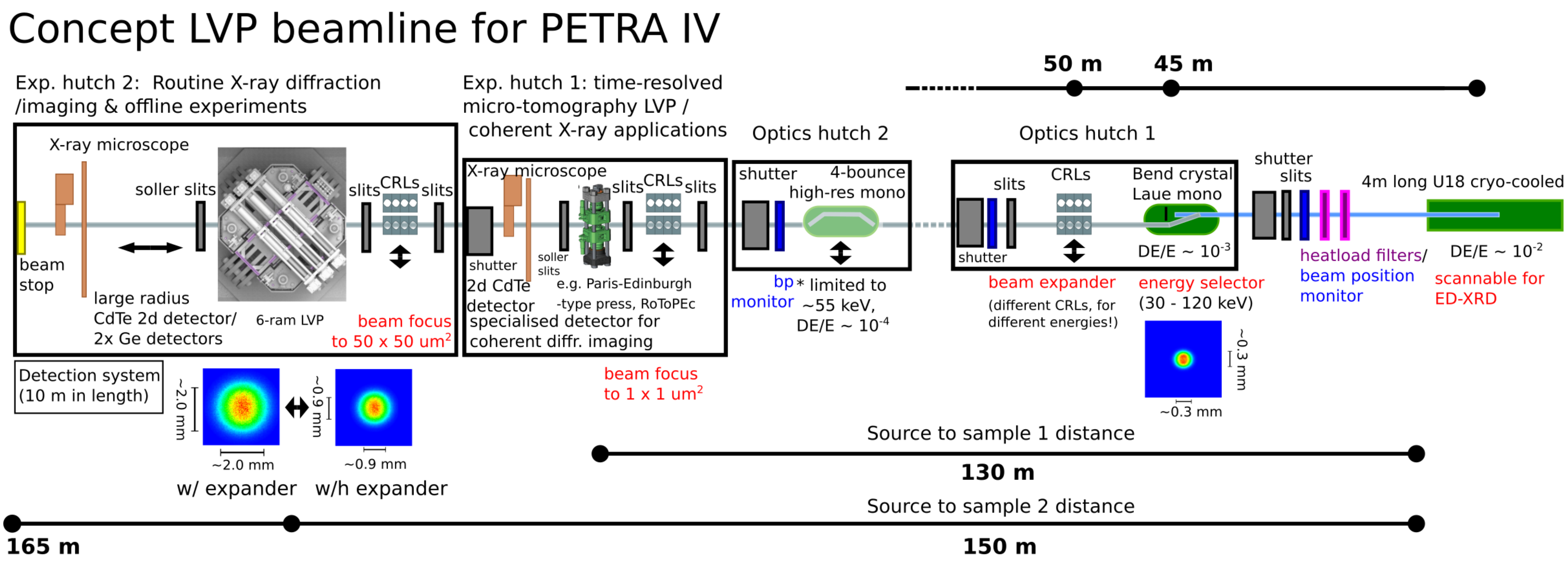


Example PETRA IV beamline for LVPs

Concept LVP beamline for PETRA IV

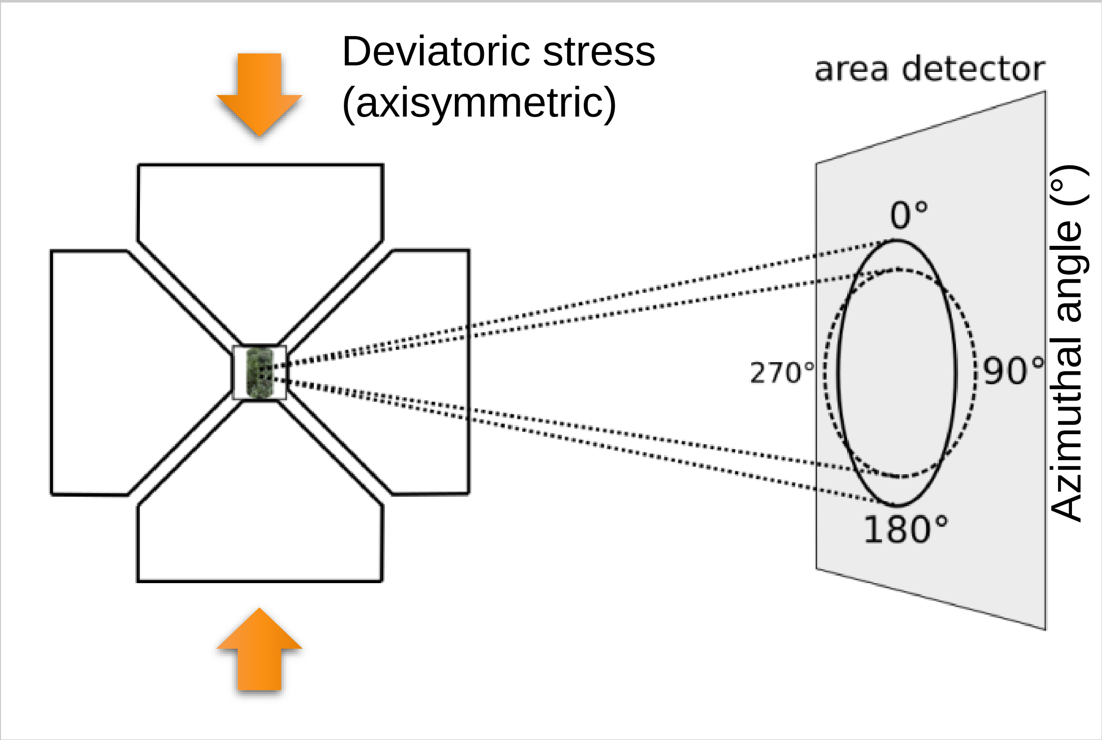


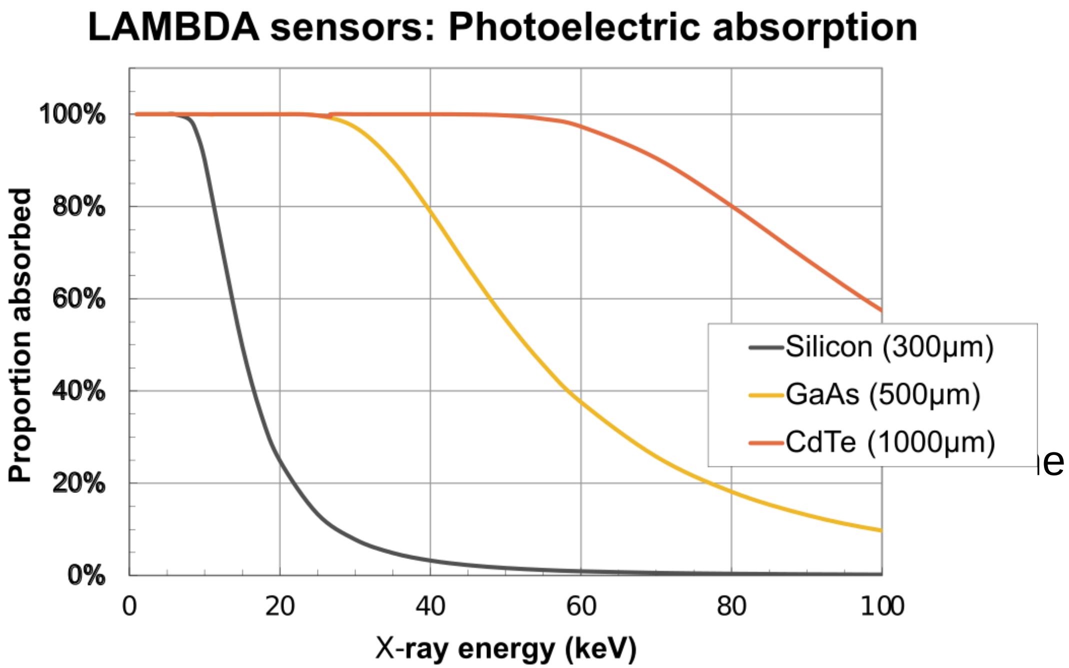
Example PETRA IV beamline for LVPs



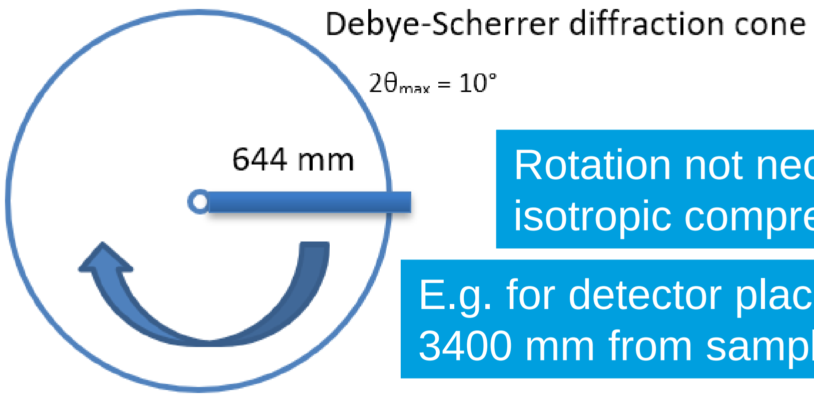
AD-XRD at PETRA IV

AD-XRD environment. Detectors.





Option for **rotating linear CdTe detector (photon-counting) on goniometer and stages** and/or **integrating 2d detectors (one or multiple panels)**



Rotation not necessary for MA6-8, isotropic compression experiments.

E.g. for detector placement 3400 mm from sample.

Summary for X-ray techniques to reach the science goals

Planned used techniques (green = full support, gold = needs more development)

X-ray diffraction techniques
- **AD-XRD for powder / single crystal**
- **Scattering on amorphous and liquid materials**
- **ED-XRD by scanning undulator harmonics**
- Other?

X-ray Imaging Techniques
- **Radiography (absorption contrast)**
- **Phase contrast imaging**
- **Time-resolved 3-D micro-tomography**
- **Near-field and far-field High-Energy Diffraction Microscopy (HEDM)**
- **Coherent Bragg-Diffraction Imaging (CDI)**
- **Scanning transmission X-ray microscopy**
- Other (?)

Spectroscopy
- Any?

What should we aim for at a high P & T LVP instrument(s)?

- High-flux, high-energy (monochromatic) X-rays: **30 – 100 keV using bent crystal Laue Mono.**
- Fast detection, high pixel resolution**: state-of-the-art CdTe detector(s)**
- Option for **scanning of harmonics** to perform **ED-XRD** (30-120 keV)
- Ample space for complementary *in situ* sample environments / measurement systems

General purpose XRD/imaging set up for low to ultra-HP experiments in **6-ram LVP**
→ fast switching between 'diffraction mode' and 'imaging mode', axial deformation mode, studies on solids

Specialized XRD/imaging/microtomography for low to moderate P and T experiments in **PE-press(es)**
→ fast switching between 'diffraction mode' and 'imaging mode', torsion deformation mode, studies on liquids

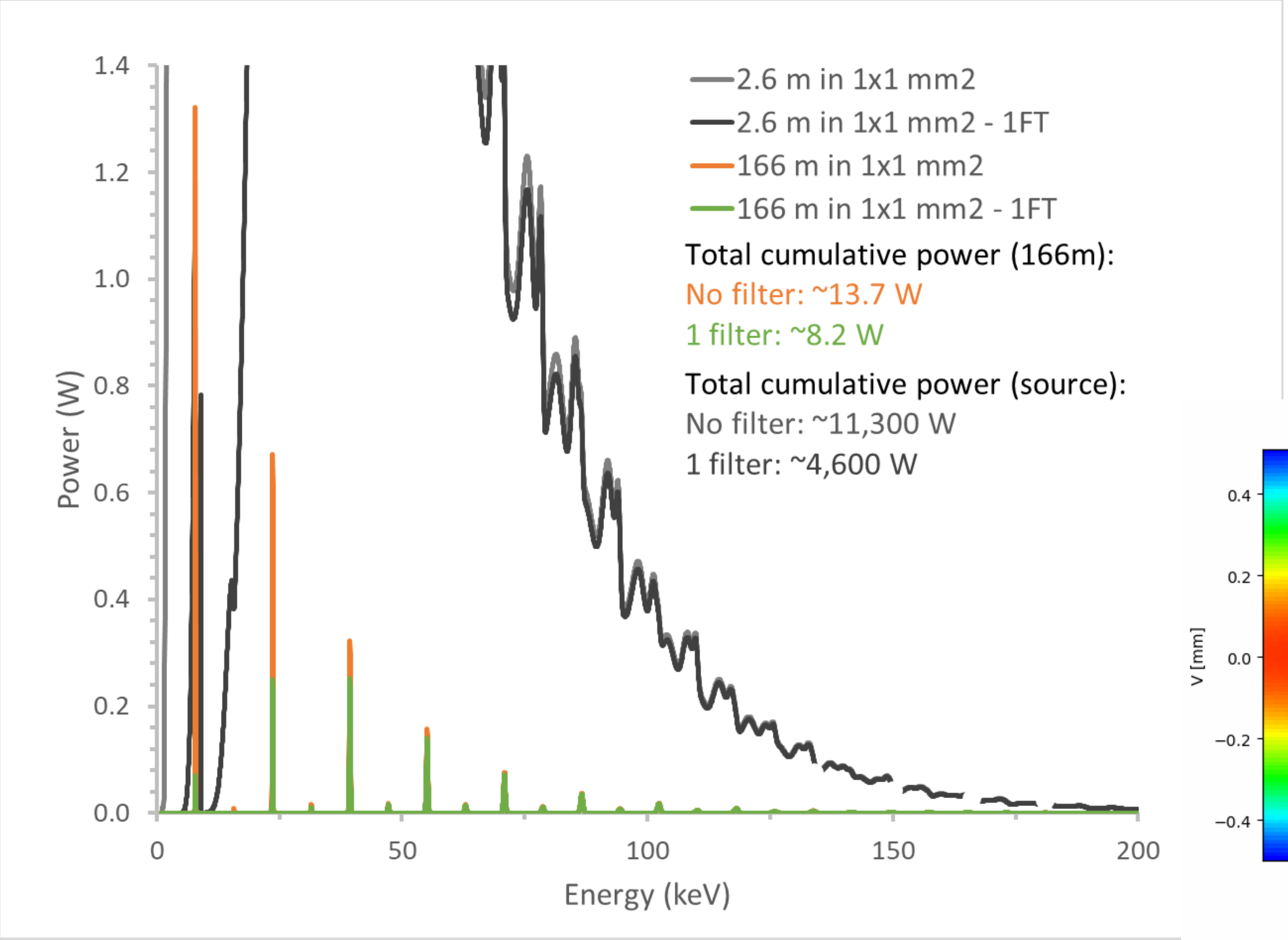
Outlook

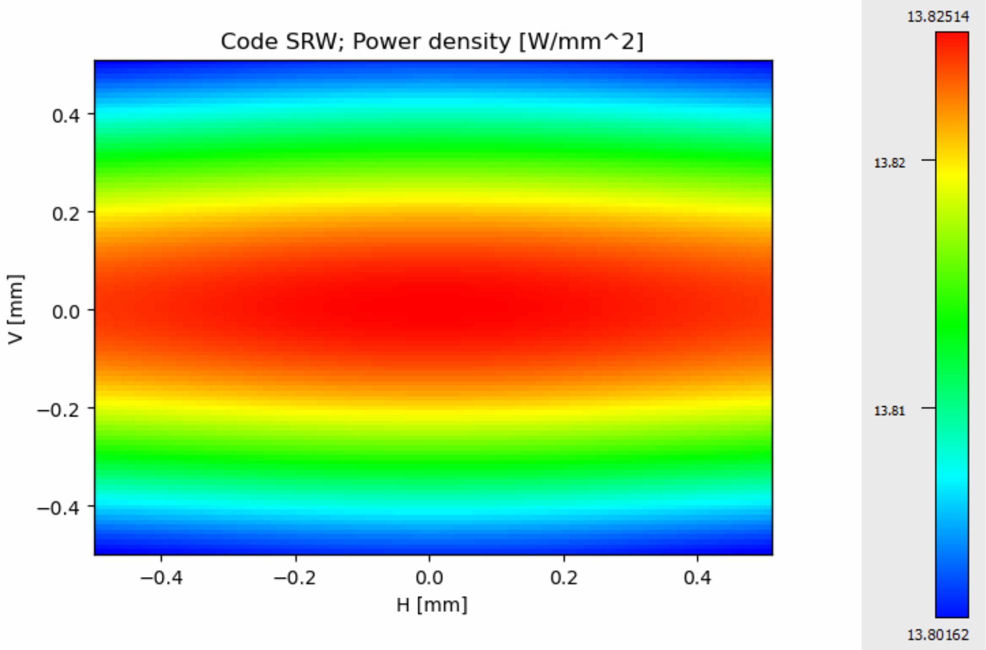
- **Next few weeks, last chance to review and comment on SIPs!!**
- **All participants in the LVP@P4 workgroup please indicate which proposals you will support and sign.**
  - **Email Dr. Melanie Sieber your preference!**
- **Finalized proposals**
  - ***To be circulated on various mailing lists to seek out more signatures (?)***
  - **To be submitted before the deadline (1 Dec 2020) by Dr. Sieber**

Thank You for Your Attention!

Power

Calculations of undulator power (density) at beamline U61 (166 m from the source)





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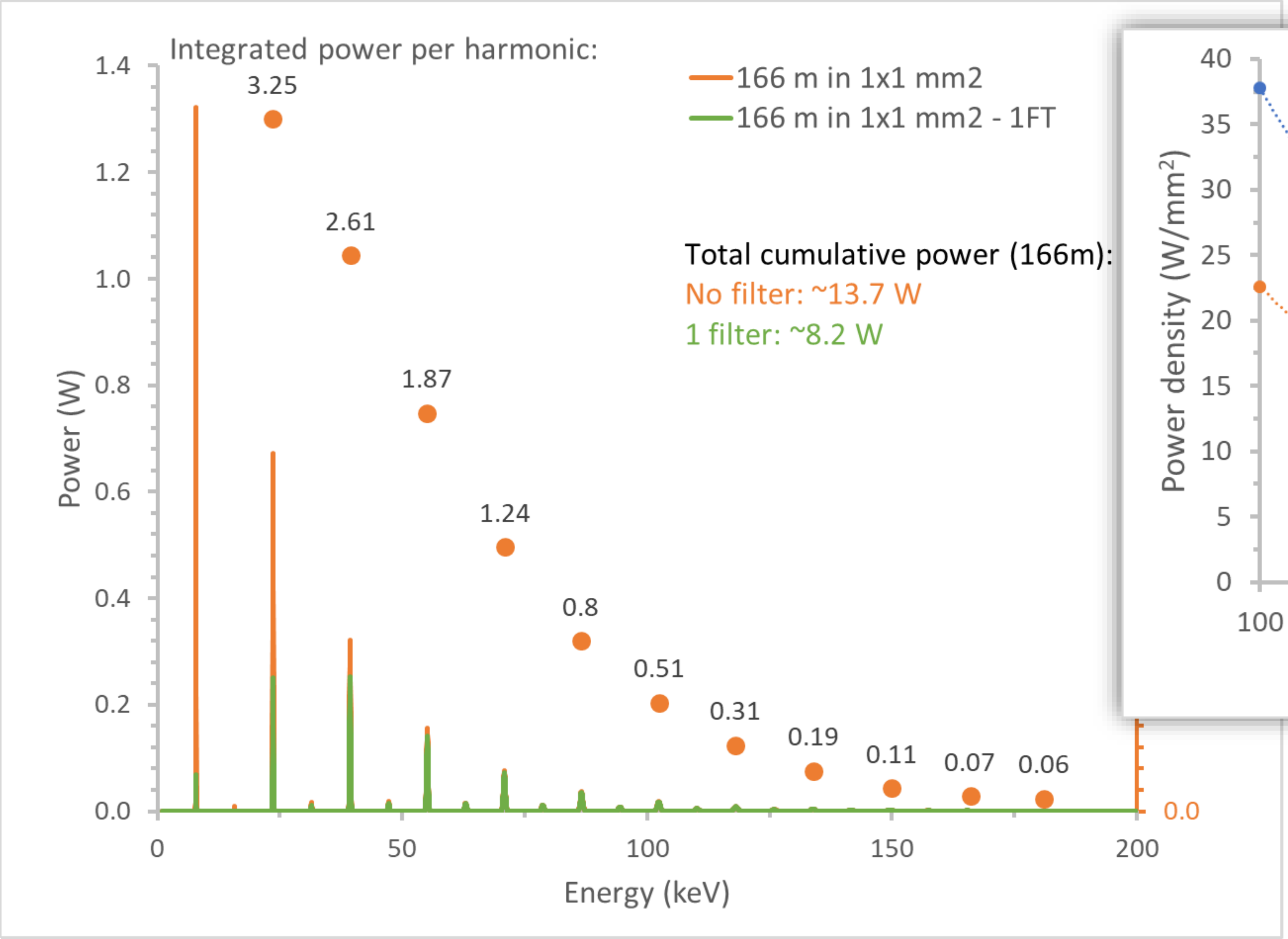
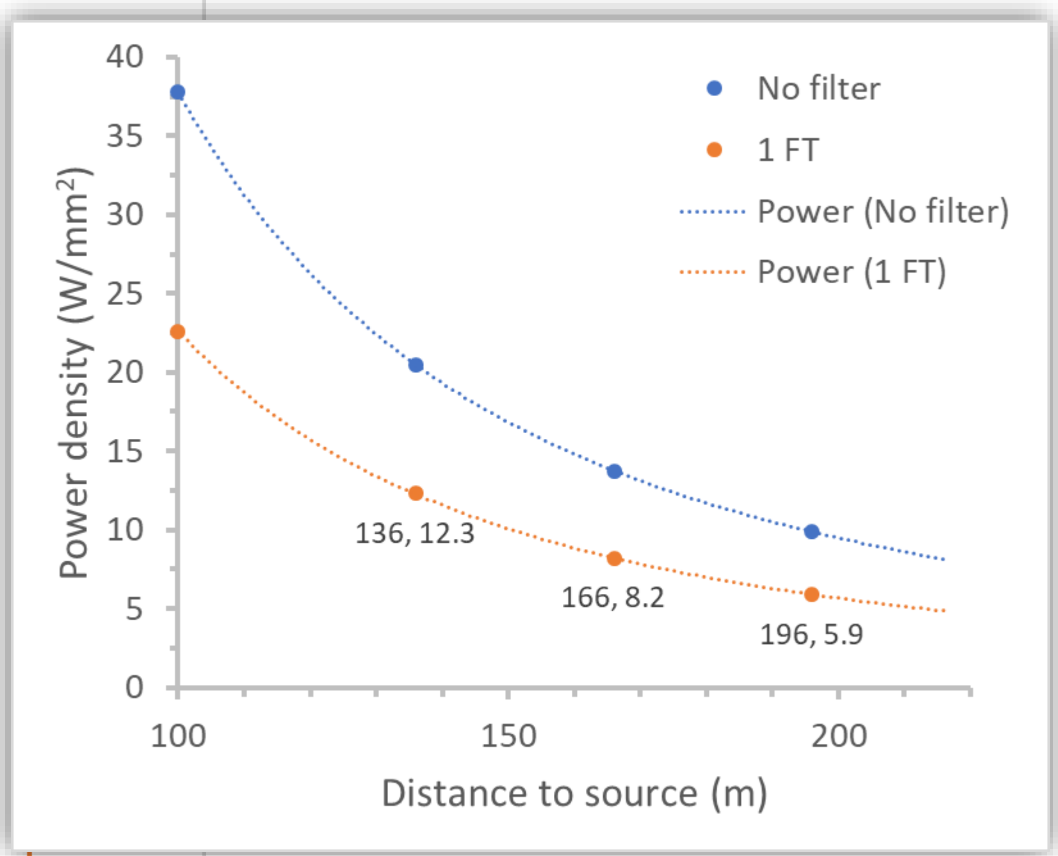
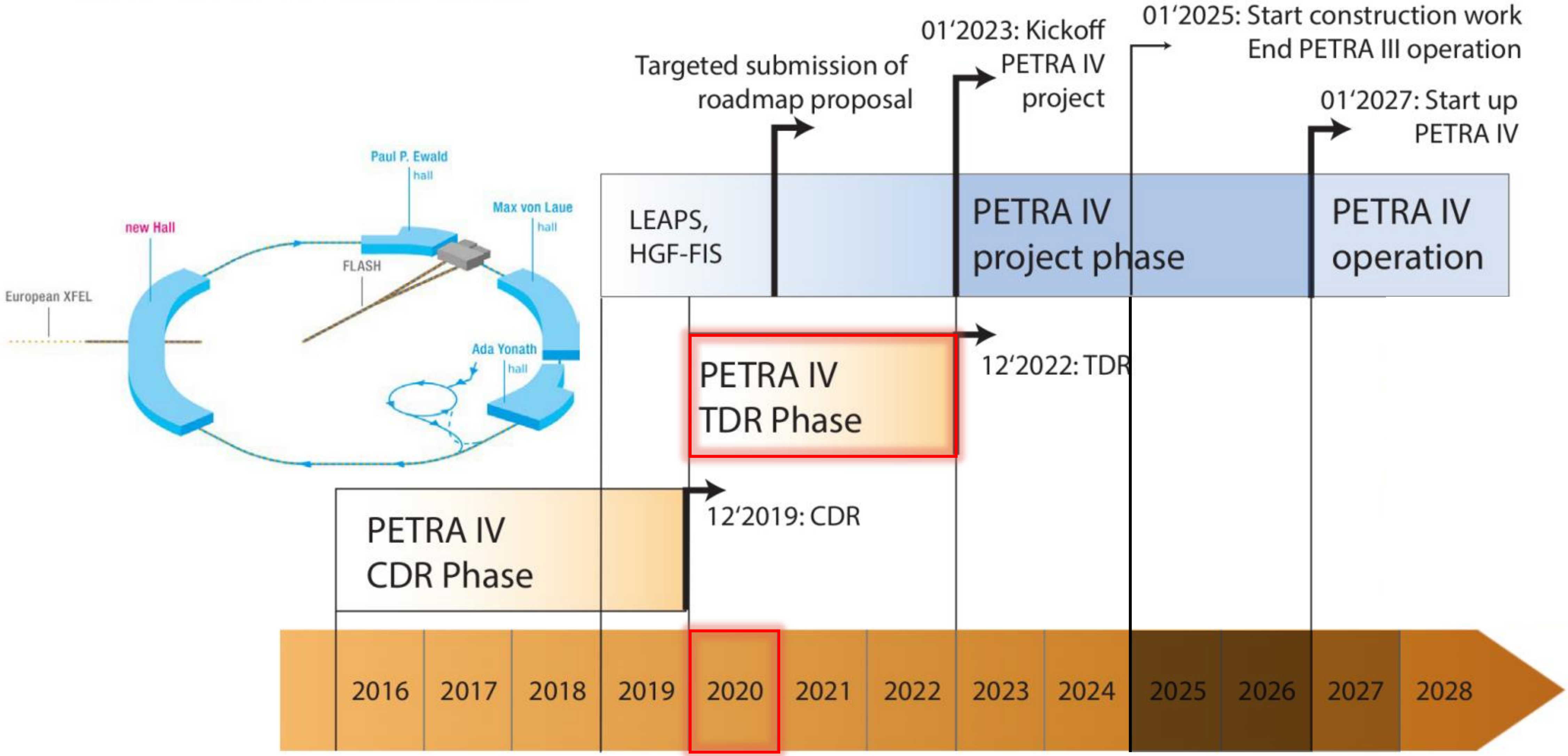




Total power density of all harmonics as function of distance

Outlook of PETRA IV.

Task ahead: From Idea to Reality



Outlook of PETRA IV.

Work packages

Work Package Group 3: Photon Science Experiments

FS

- WP 3.01: X-Ray Sources
- WP 3.02: Front-End Optics & Monochromators
- WP 3.03: Ultraprecision Mechanics
- WP 3.04: Nano-Optics
- WP 3.05: Data Management and Analysis
- WP 3.06: Technical Infrastructur Design
- WP 3.07: Sample Environments and User Laboratories

WP 3.08: Beamline and Experiment Design

Topics:
Energy
Life and Health
Transport and Technology
Earth and Environment
Industrial Innovation
Nano and Quantum Materials for Information Technology

- Flagship Beamline: U01
- Flagship Beamline: U21
- Flagship Beamline: U31
- Flagship Beamline: U41
- Flagship Beamline: U61
- Upgrade Beamline: U02
- Upgrade Beamline: U03
- Upgrade Beamline: U22
- Upgrade Beamline: U42

WP 3.08: Beamline and Experiment Design

Topics:
Energy
Life and Health
Transport and Technology
Earth and Environment
Industrial Innovation
Nano and Quantum Materials for Information Technology

6 Workshops planned from September 2020!

Beamline proposals for portfolios to guide TDR must be ready in 6 months!

→ First report due in May 2020!
→ 1st meeting in February with P02.2

- **What design LVP beamline do we want and need?**
- **Core driver experiment for U61?**
- **An independent beamline (100%), more than 1 beamline?**

Contact

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