NMX Instrument Design and Expected Performance

NMX STAP

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High-level Requirements – starting point

- A typical system to be studied would be a 30-40 kDa protein
- Unit cell edges 100-150 Å, up to 300 Å
- Realistic dmin ~1.8 Å, rarely < 1 Å
- Crystal size ~0.01-0.1 mm3
- Data set in one day

High-level Scientific Requirements

1. The instrument shall allow data collection from crystals with unit cell repeats > 300 Å.
2. The instrument shall allow data to be collected to a dmin of 1.5 Å.
3. The instrument shall match the size of the neutron beam to the size of the sample.
4. The instrument shall match the divergence of the neutron beam to the mosaicity of the sample.
5. The instrument should maximise the signal-to-background (S/B) ratio of the Bragg reflections.
6. The instrument should allow data collection from crystals of < 0.01 mm3 volume

Choice of wavelength range

Cold

- ☺Higher scattering efficiency
- ☺Better detector efficiency
- ☺Reflections better separated in 2θ
- ☹d_{min} limited to ½λ
- ☹Small Ewald sphere → large blind area

Thermal

- ☺Higher flux at short λ
- ☺More reciprocal space coverage in the same solid angle
- ☹Reflections more difficult to separate on the detector
- ☹Detector efficiency can become a problem

Instrument length and wavelength band

How to resolve reflections with a long pulse?

By time-of-flight

☺Lower spatial resolution needed on the detector → can use existing technology

☺Can accept more divergence

☺Wider wavelength band

☹Need to chop the pulse → ~90 % loss in flux + cost of chopper (~1 M€)

On the detector plane

☺Can use full pulse

☺No need for high timing resolution (~1 ms is OK)

☹Detector technology does not exist yet (can be expensive)

☹Narrower wavelength band

NMX – conceptual view

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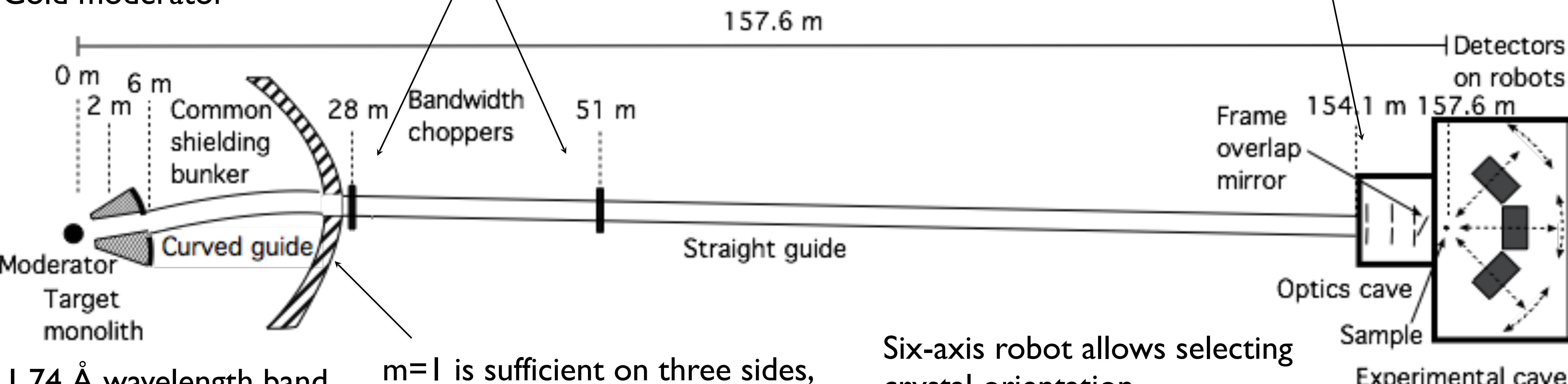
Adjustable opening chopper allows flexible bandwidth selection.

Collimation section giving flexibility in beam size and divergence

Cold moderator



1.74 Å wavelength band (1.8-3.55 Å)

m=1 is sufficient on three sides, m=2.2 for curving

Six-axis robot allows selecting crystal orientation

Three 60 x 60 cm detectors with 0.2 mm spatial resolution Variable sample-detector distance (0.2-1.0 m)
Variable 2θ angle (0-110°)

- **NMX** @ ESS, Lund, Sweden
  - Cold, TOF-Laue, Δλ<1.75 Å
  - 158 m length, λ-range 1.8-10 Å
  - Flexible geometry (robots)
  - Gd-GEM detector

Flux at sample – time averaged

- By Monte Carlo simulation 2×10^9 n/s/cm^2 at ±0.2° divergence
- LADI-III 5×10^7 n/s/cm^2, divergence unclear

Factor 40

- PCS 9.7×10^6 n/s/cm^2 at ±0.1° divergence

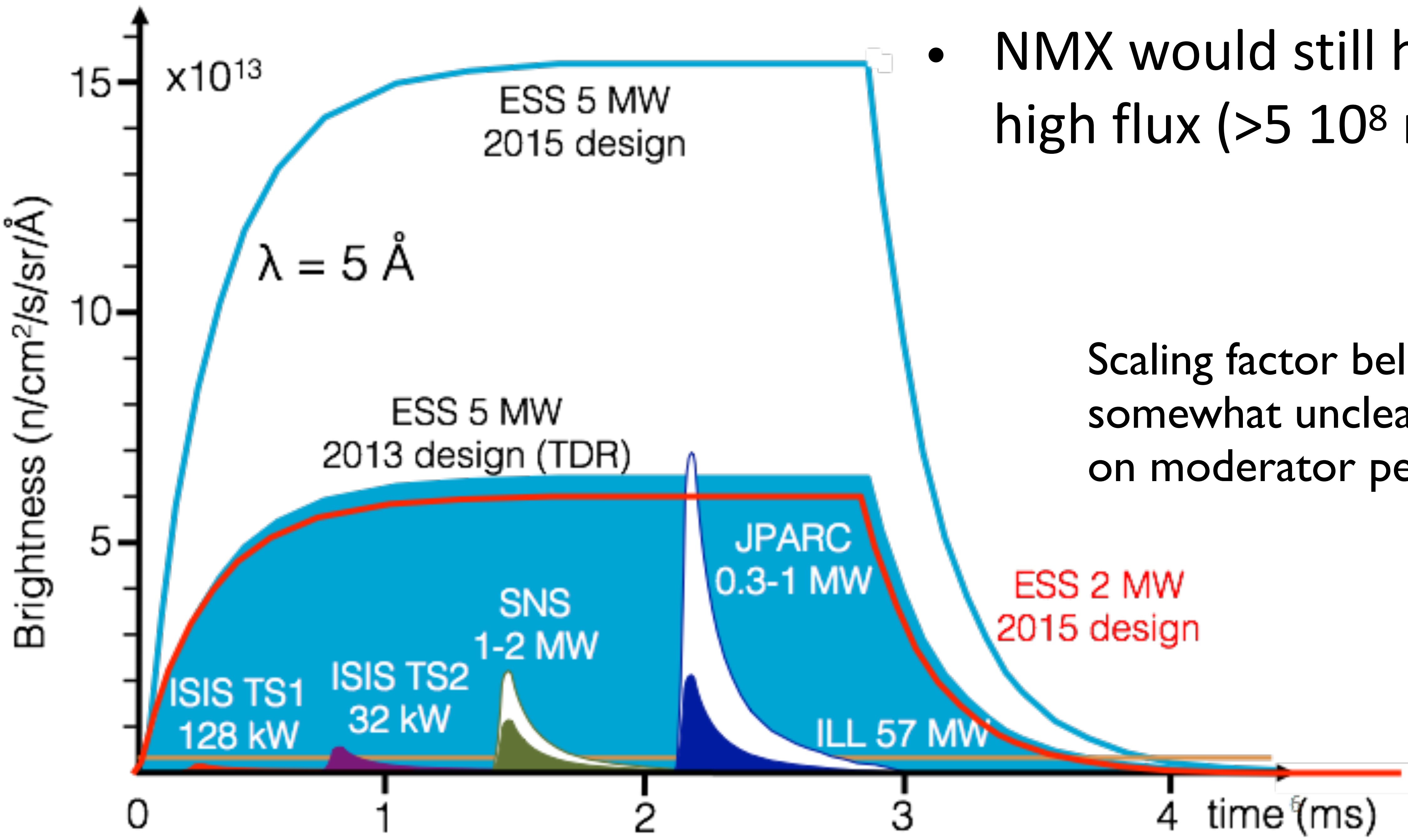
Factor 200

NMX makes full use of the long pulse and high-brilliance moderators

The instrument should allow data collection from crystals of < 0.01 mm3 volume

Should be realistic to collect 0.1 mm^3 crystal in < 1 day

Operation at 2 MW



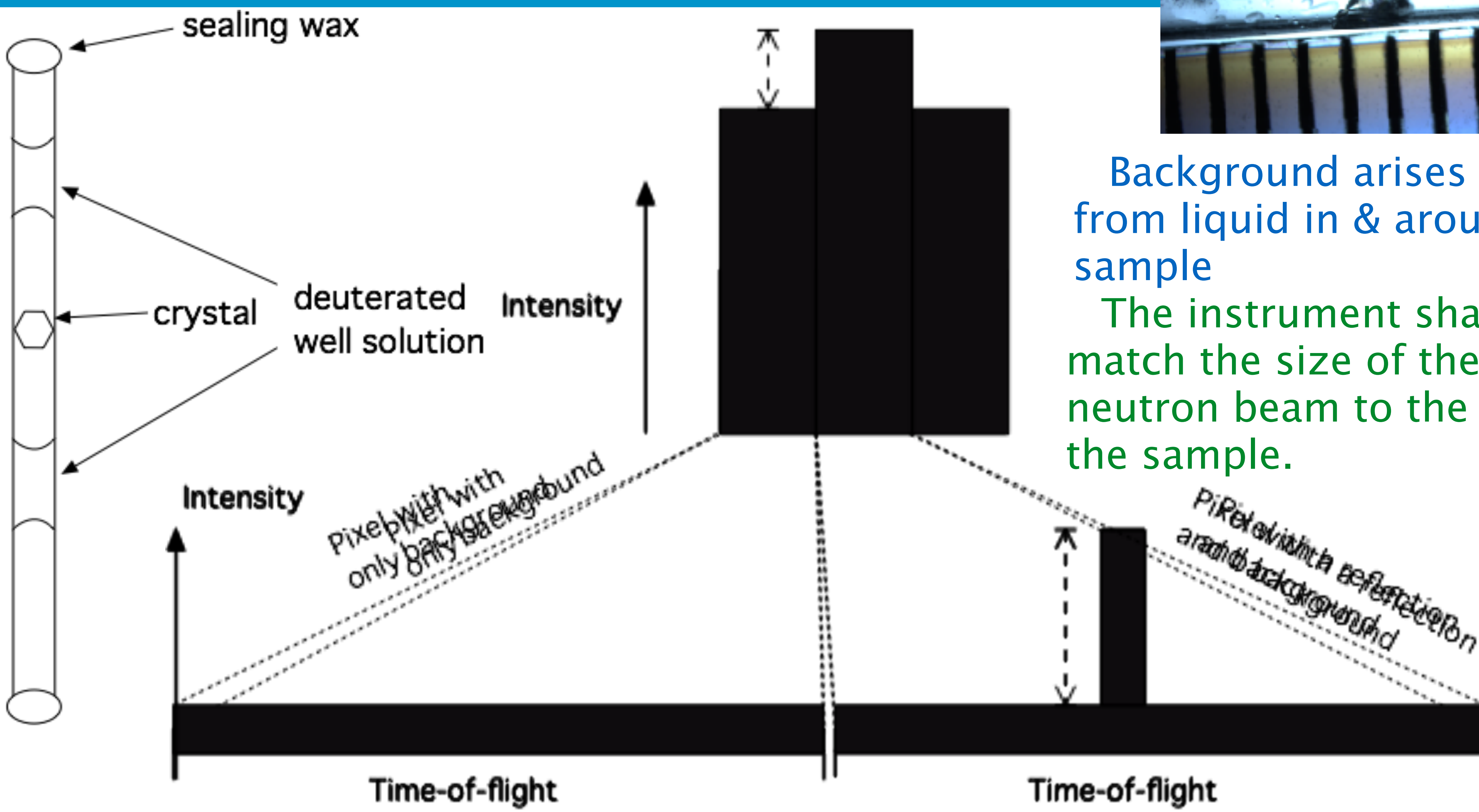
- Factor 2-3 in flux vs. 5 MW
- NMX would still have very high flux (>5 10^8 n/s/cm^2)

Scaling factor below 2 MW somewhat unclear; depends on moderator performance

Spreading background over time-of-flight

Background arises mostly from liquid in & around the sample

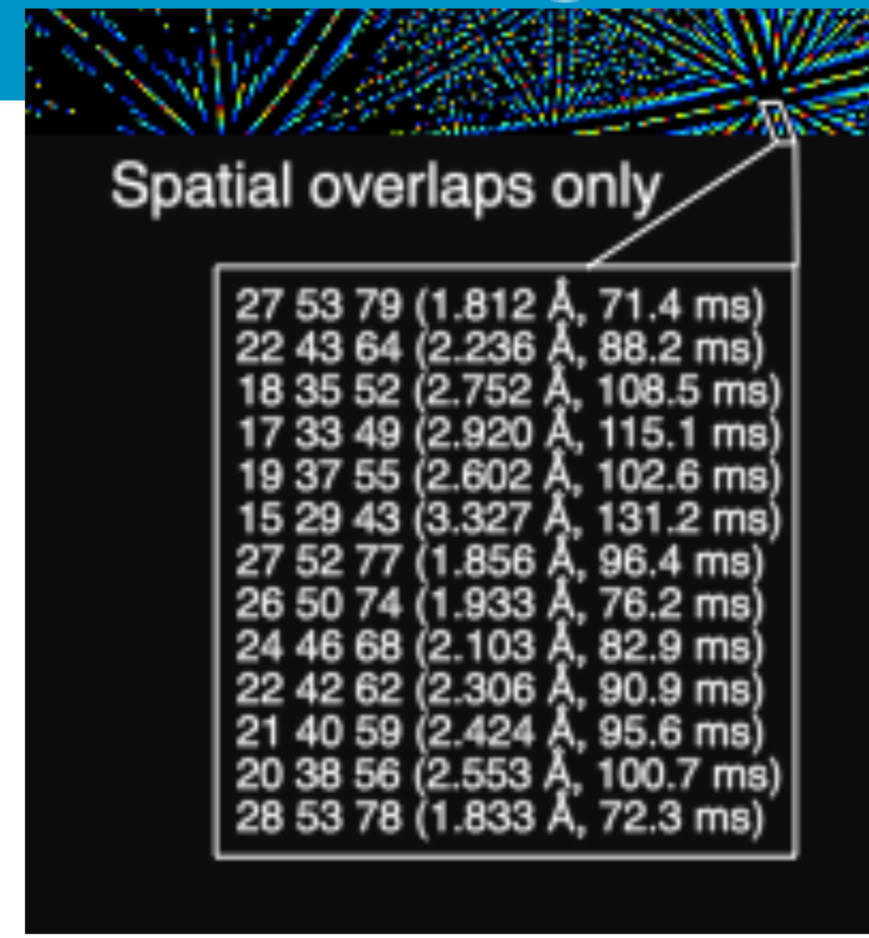
The instrument shall match the size of the neutron beam to the size of the sample.

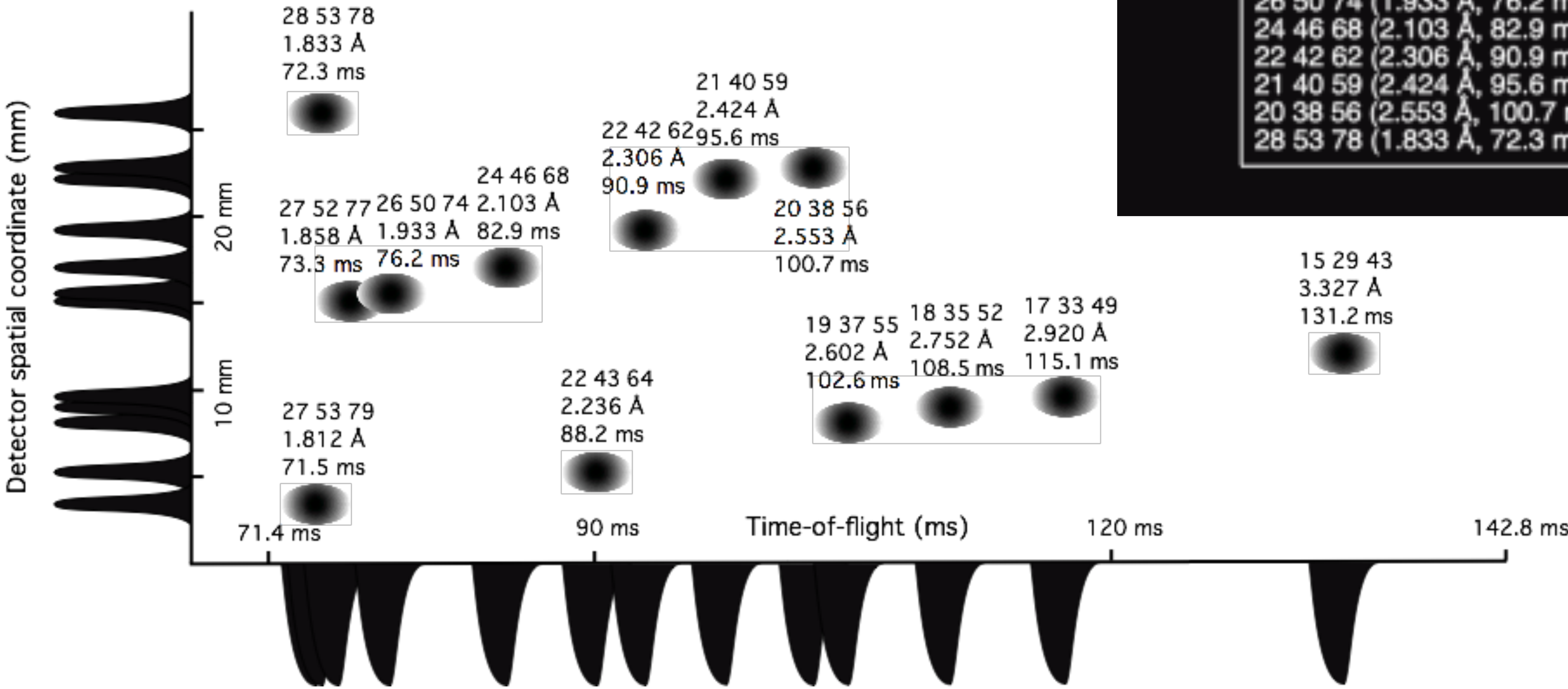


Signal/background gain from TOF is difficult to quantify – depends on crystal

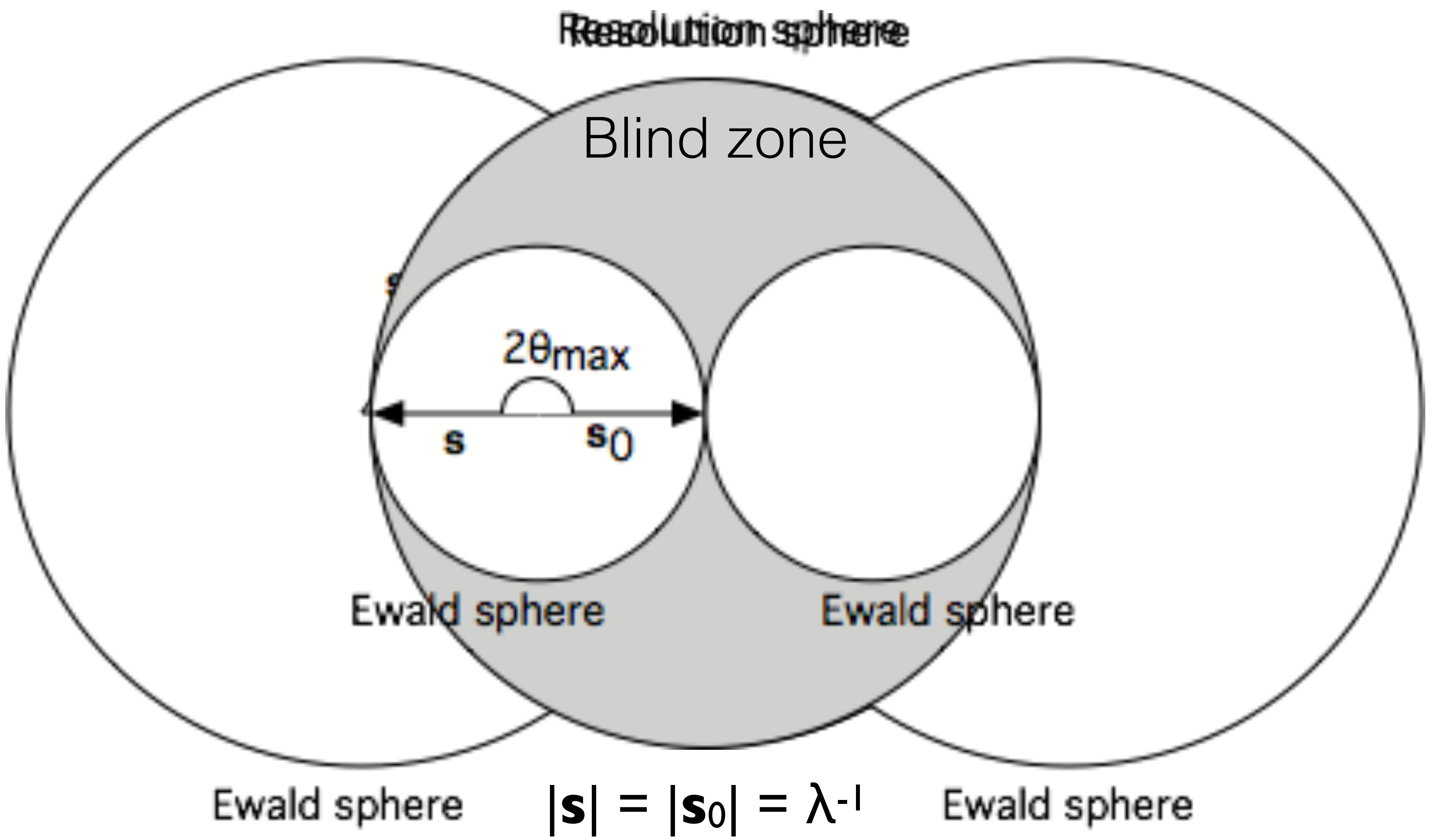
Overlap separation with TOF

The instrument shall allow data collection from crystals with unit cell repeats > 300 Å





Completeness problem with long wavelengths



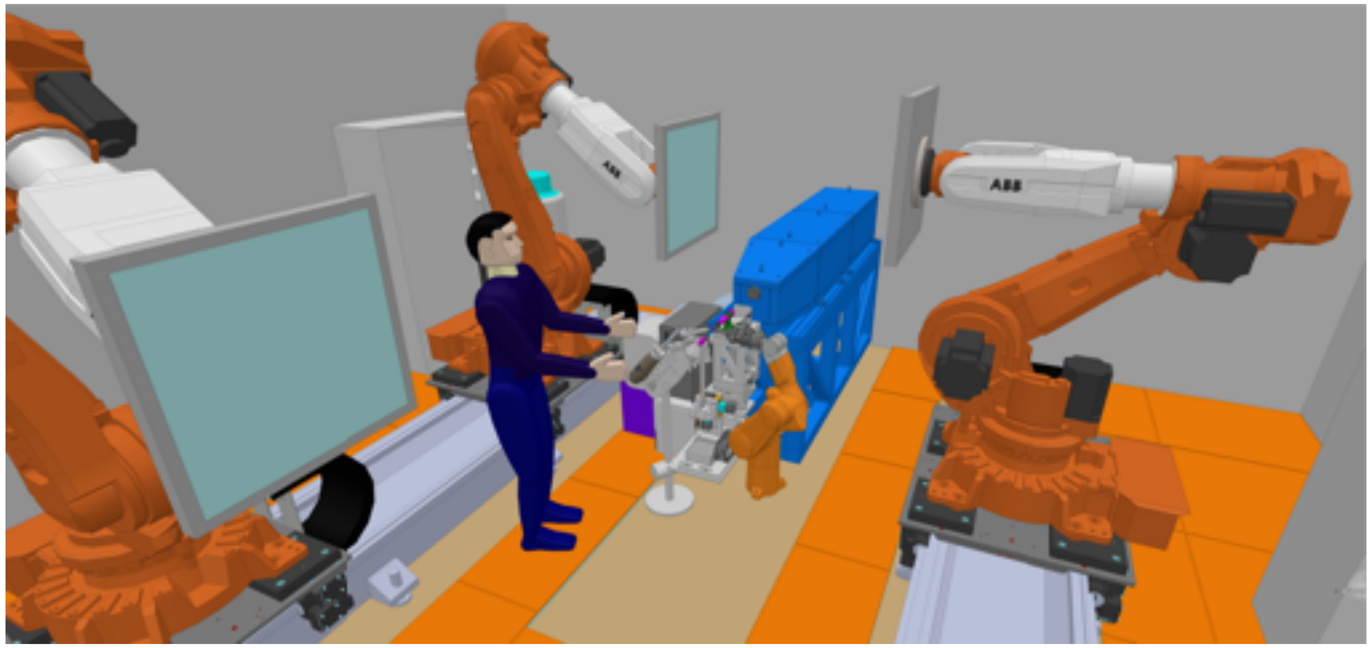
Multi-axis goniometry

Large solid angle detectors

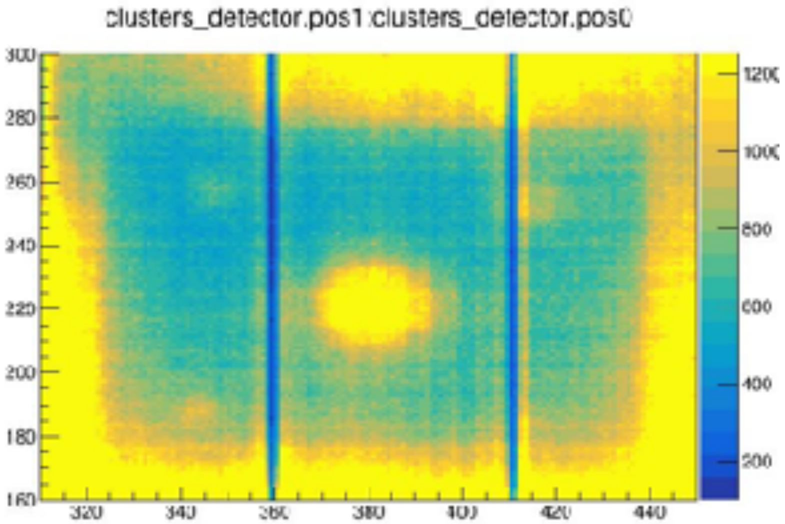
The instrument shall allow data to be collected to a d_{min} of 1.5 Å

- Scattering power increases with wavelength
- Air scattering/ absorption is not a problem with neutrons
- Long wavelengths require large 2θ
- Blind zone gets large

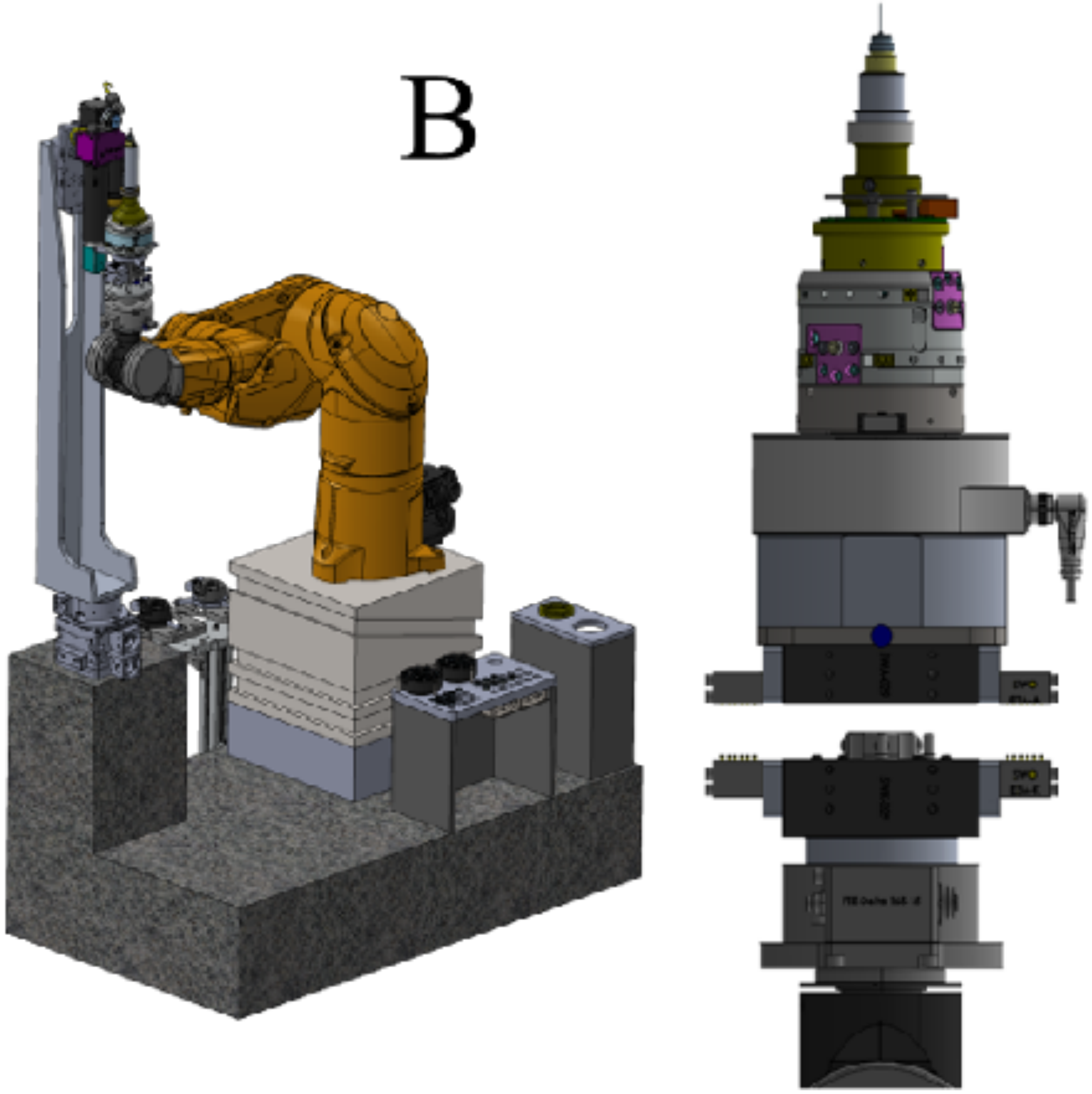
Endstation – Robotics



Large solid angle detectors



50 x 50 cm, effective pixel size 400 µm



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Multi-axis goniometry

Crystal size or collection time?

The instrument should allow data collection from crystals of < 0.01 mm3 volume

Should be realistic to collect 0.1 mm^3 crystal in < 1 day

1. Do we want to push minimum crystal size and collect data for weeks?
2. Do we want to push unit cell size and collect data for weeks (on a large crystal)?
3. Do we want to push throughput and collect data in a day from larger crystals? Software!

Choice not limited by design decisions

Software & instrument throughput

- Data collection strategy software can save significant beamtime (or get better completeness in the same time)
- Work flow automation can save considerable time when testing larger numbers of crystals (e.g. evaluate resolution from test images)

Conclusion

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- No compromises in performance were necessary when going from preliminary to detailed engineering design
- Design allows choices between capability and capacity

Questions?

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