NMX – Macromolecular crystallography

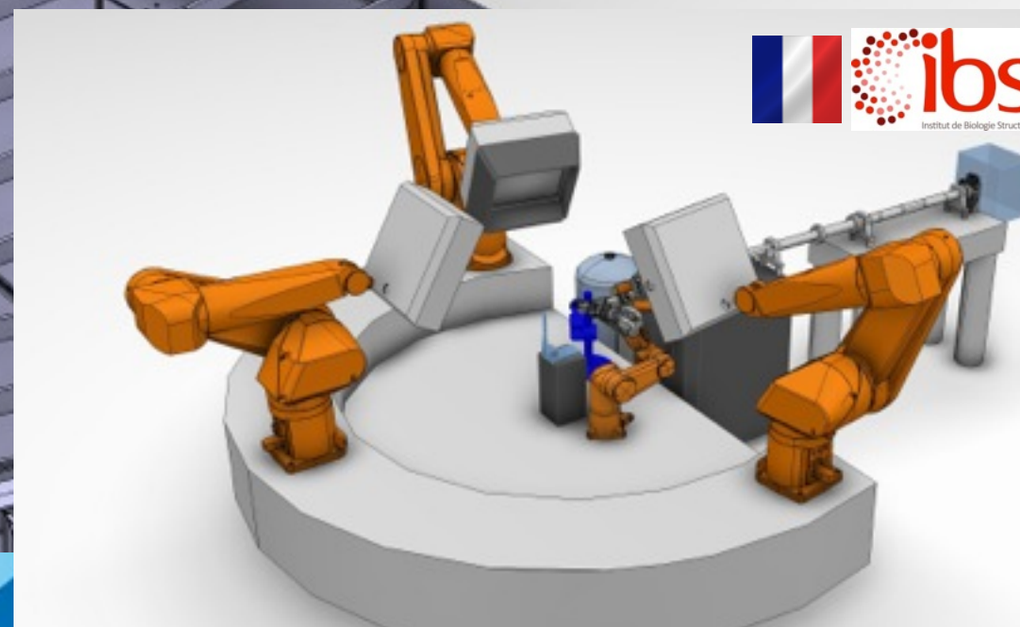
Partners

Key advantages of ESS Macromolecular Diffractometer

Smaller crystals needed (200 µm vs. 1 mm)

Data collection faster (days vs. weeks)

Larger unit cells possible (300 Å vs. 150 Å)



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 d_{min} of 1.5 Å. → λ =1.8-3.55 Å
- 3. The instrument shall match the size of the neutron beam to the size of the sample. → 0.2 - 5 mm
- 4. The instrument shall match the divergence of the neutron beam to the mosaicity of the sample. → ±0.2°
- 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 mm^3 volume

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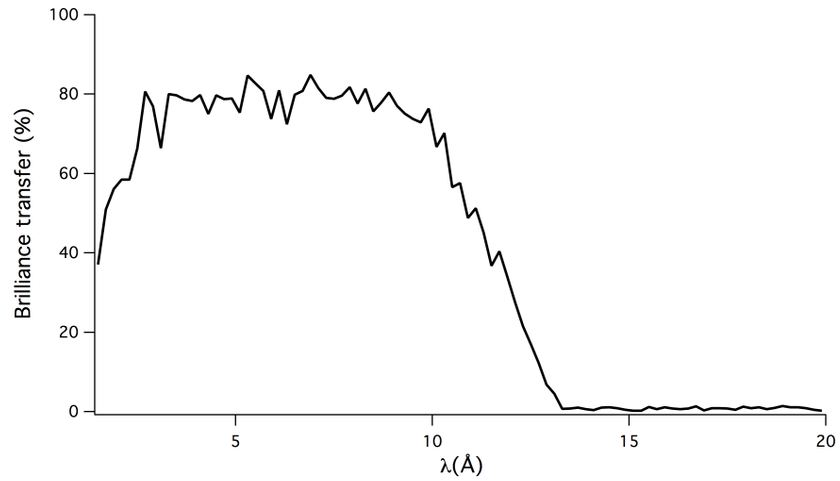
Optics overview

Curved inside bunker, optimised for maximum brilliance transfer at 2Å



- Monolith insert horizontally straight, vertically tapers from 31 mm to 46 mm, m =2 horizontal, m = 1 vertical
- 1.2 km curvature radius within bunker
- m = 2.2 on the curve, otherwise m = 1
- Line of sight lost at 31.5 m from the moderator
- Straight guide up to 154.1 m from the moderator, m = 1
- Frame overlap mirror for λ > 10 Å

Optics concept choice – pros

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Option 4: Curved inside bunker, optimised for maximum brilliance transfer at 2Å

- Acceptable performance for ±0.2° divergence at < 2 Å
- Good performance all round for ±0.1° divergence – this range is more typical for experiments
- Loss of line-of-sight almost within bunker – lower shielding cost & easier component maintenance
- Deflects the beam far enough from the sector centreline to allow two beams to be extracted from the same beamport

Updating optics concept to empty bunker

- 2x LOS no longer relevant – how much do we need to curve?
- Even more important to get out of direct fast beam within bunker!
- Misalignment issues possible with 30x30 mm guide – can we expand long straight section?
- Can avoid optics in monolith insert?