NMX Instrument Overview & Staging Plan

Esko Oksanen
Scientific Project Leader

Giuseppe Aprigliano
Lead Instrument Engineer

NMX Tollgate 2 Review

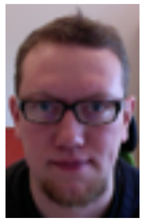
2014-12-11

Outline

- **Instrument concept and scientific case** EO
- Key components overview EO
- Scientific scope coverage EO
- Layout GA

NMX Instrument team

Scientific Project Leader



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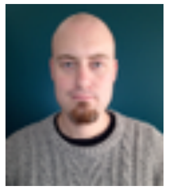
Lead Instrument Engineer

Giuseppe Aprigliano

Neutron Optics and Shielding

Valentina Santoro



Phillip Bentley

Damian Martin-Rodriguez

Neutron Choppers

Iain Sutton

Markus Olsson

Motion Control & Automation

Thomas Gahl

Paul Barron

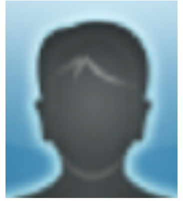
Neutron Detectors

Richard Hall-Wilton

Dorothea Pfeiffer

Data Management & Software Center

Thomas Holm Rod

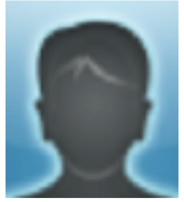


Jonathan Taylor

Planning office

Magnus Israelsson

Systems Engineering Support



Peter Sångberg

Scientific Partners

ibs Institut de Biologie Structurale

Centre for Structural Biology • Aarhus University •

Scientific and Technical Advisory Panel (STAP) for Macromolecular Crystallography

John Helliwell, University of Manchester, UK — Chair

Paul Langan, ORNL, TN, USA

Sean McSweeney, BNL, NY, USA

Derek Logan, Lund University, Sweden

Matthew Blakeley, ILL, France

Nobuo Niimura, Ibaraki University, Japan

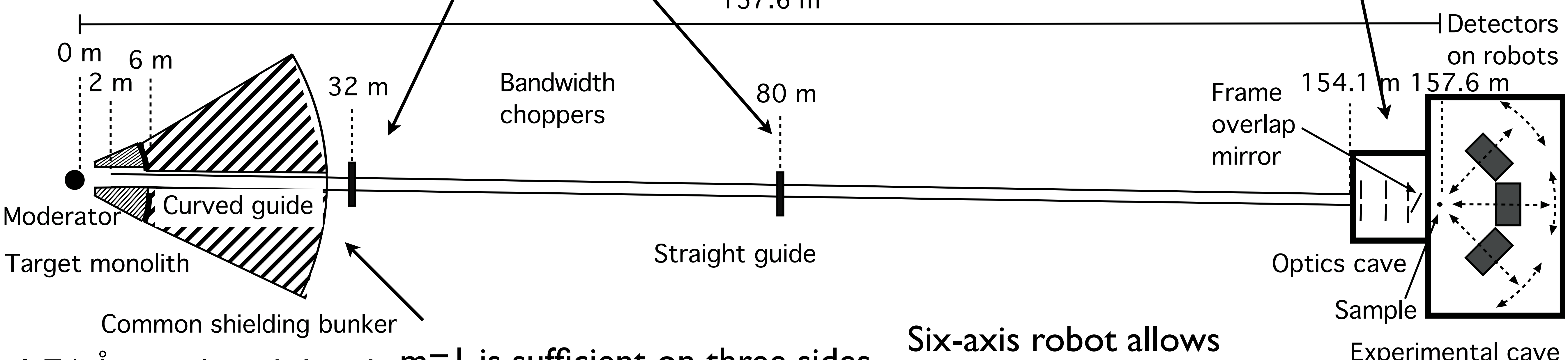
Manuel Angst, FZJ, Germany

NMX – A quasi-Laue time-of-flight diffractometer with high **q**-resolution

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°)

- Match beam size to sample size (max 5 x 5 mm)
- Match beam divergence to sample mosaicity (max. ±0.2°)
- Maximize (useful) flux at sample!

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Existing technology

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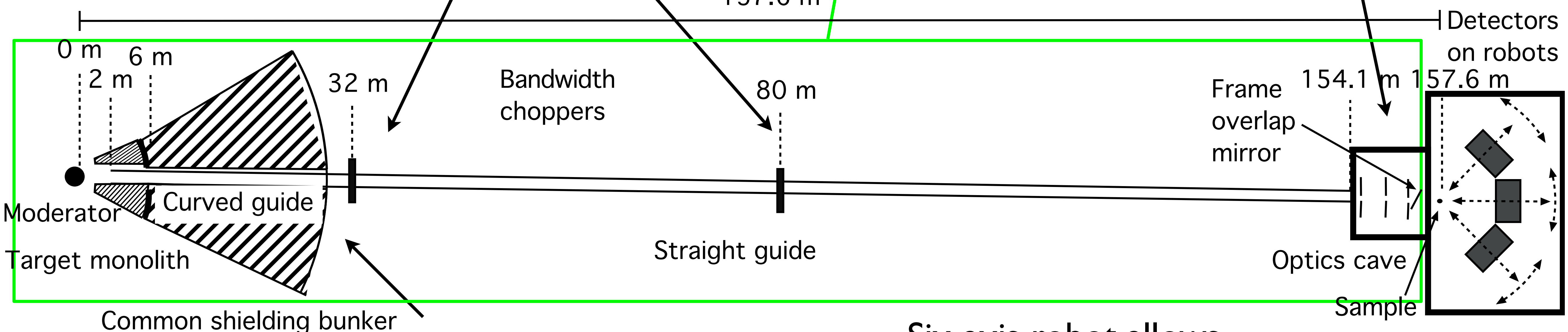

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Existing technology

Needs R&D

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Collimation section giving flexibility in beam size and divergence

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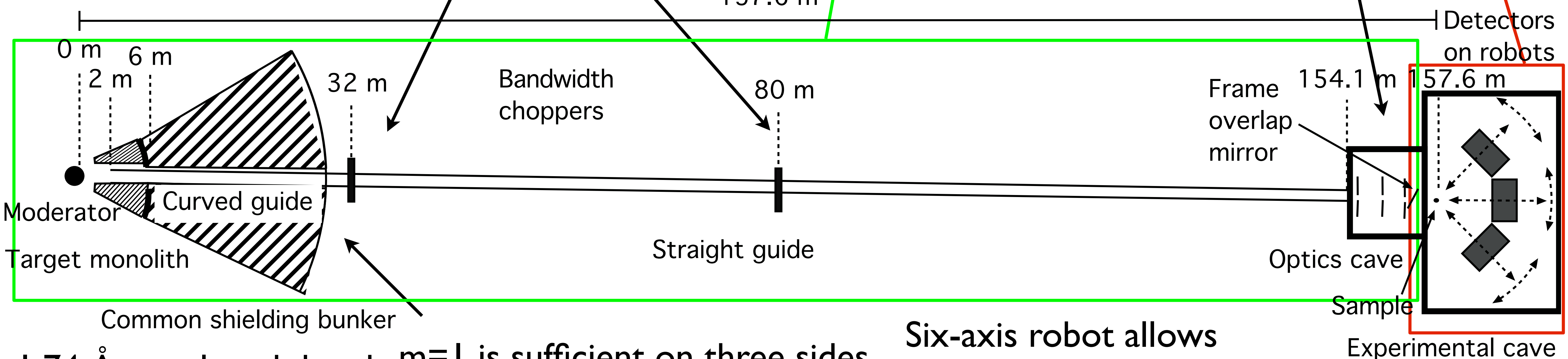

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Game-changer for neutron crystallography

Where are hydrogens important?

Enzyme mechanisms →

Protein-ligand interactions → **Drug design**

Proton transport across membranes →


The Nobel Prize in Chemistry 1988
Johann Deisenhofer, Robert Huber, Hartmut Michel

Hartmut Michel - Facts

Hartmut Michel

Born: 18 July 1948, Ludwigsburg, West Germany

Affiliation at the time of the award: Max-Planck-Institut für Biophysik, Frankfurt-on-the-Main, Federal Republic of Germany

Prize motivation: "for the determination of the three-dimensional structure of a photosynthetic reaction centre"

Field: biochemistry, structural chemistry

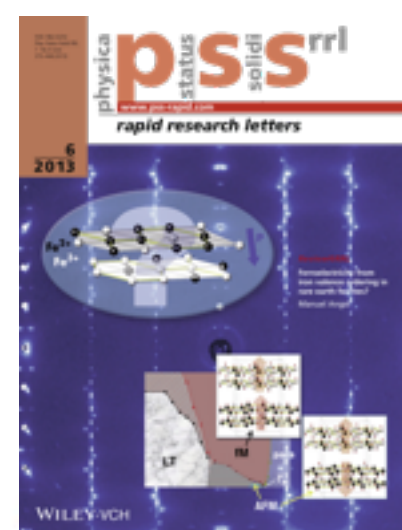
"There is no alternative to neutron crystallography in order to uniquely identify the location of protons, which is of particular importance when dealing with proton translocating proteins" H. Michel, MPI of Biophysics

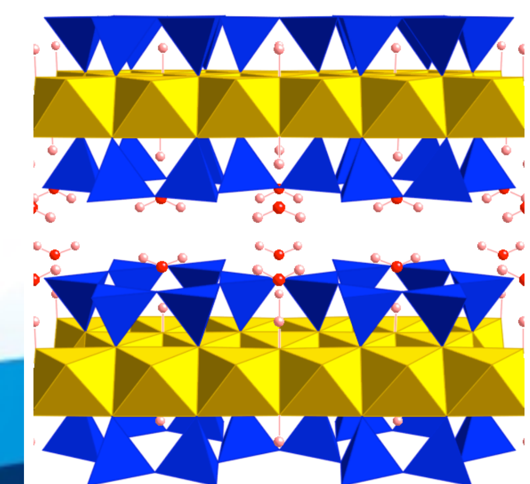
"This proposed beam line opens a wide, new field of opportunity as a state-of-the-art workhorse facility for obtaining accurate models of biological macromolecules (protein, RNA, DNA), in particular with experimentally based knowledge of the location of hydrogen atoms and therefore the fine structure of bonds, active sites and drug interactions. Furthermore, proper insight will be gained in- to water interactions – i.e. key principles of life." Prof. Poul Nissen et al., Aarhus University

Materials Science applications

Large-scale magnetic structures – Charge ordering, Ferroelectrics, Skyrmions

High-pressure, high-temperature diffraction – Hydrated phases in the Earth's mantle





Fumagalli et al. (2002) EPSL

Esko Oksanen, European Spallation Source

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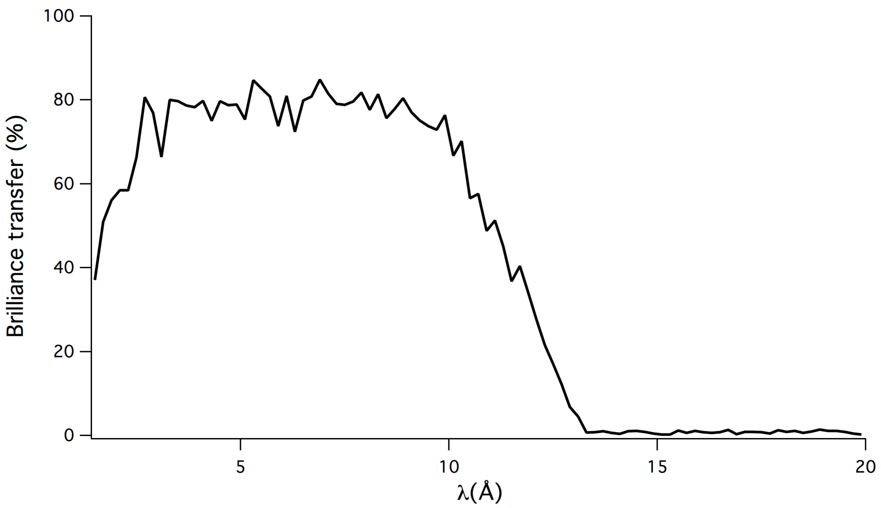
Damian Martin Rodriguez

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

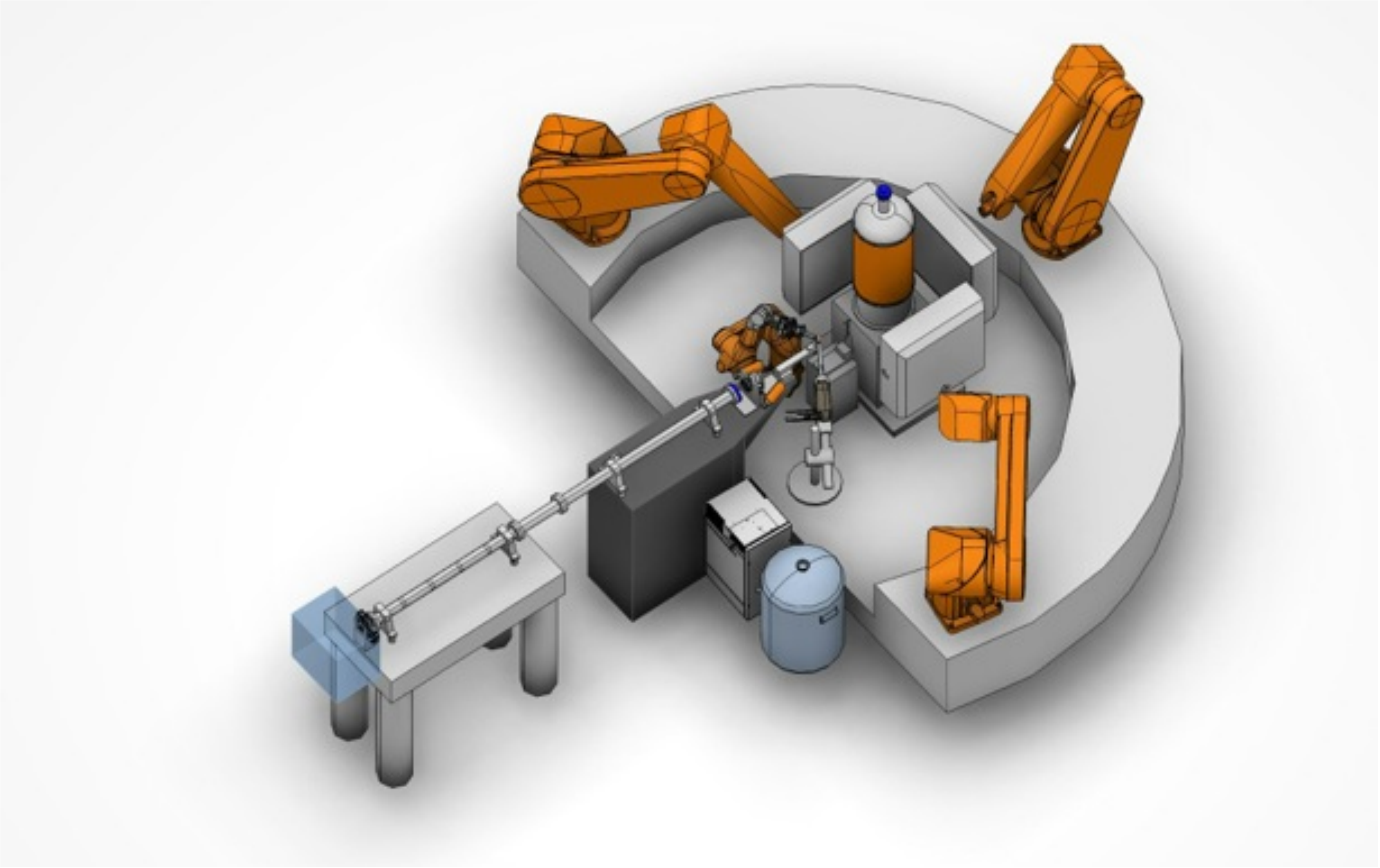
Choppers

- Choppers are for wavelength selection
- Single disc chopper at 32 m, co-rotating double disc chopper at 80 m
- Transmission has priority
- Frame overlap suppressed for λ < 12.4 Å
- Penumbra should be minimized
- No choppers in common bunker

Always 14Hz

Control bandwidth by change of phase and variable openings

Detector geometry



Robotic goniometer allows choice of sample rotation axis direction

Three 60 x 60 cm detectors with 0.2 mm spatial resolution
Sample-detector distance (0.2-1.0 m) and 2θ angle (0-110°) variable by robotic positioning

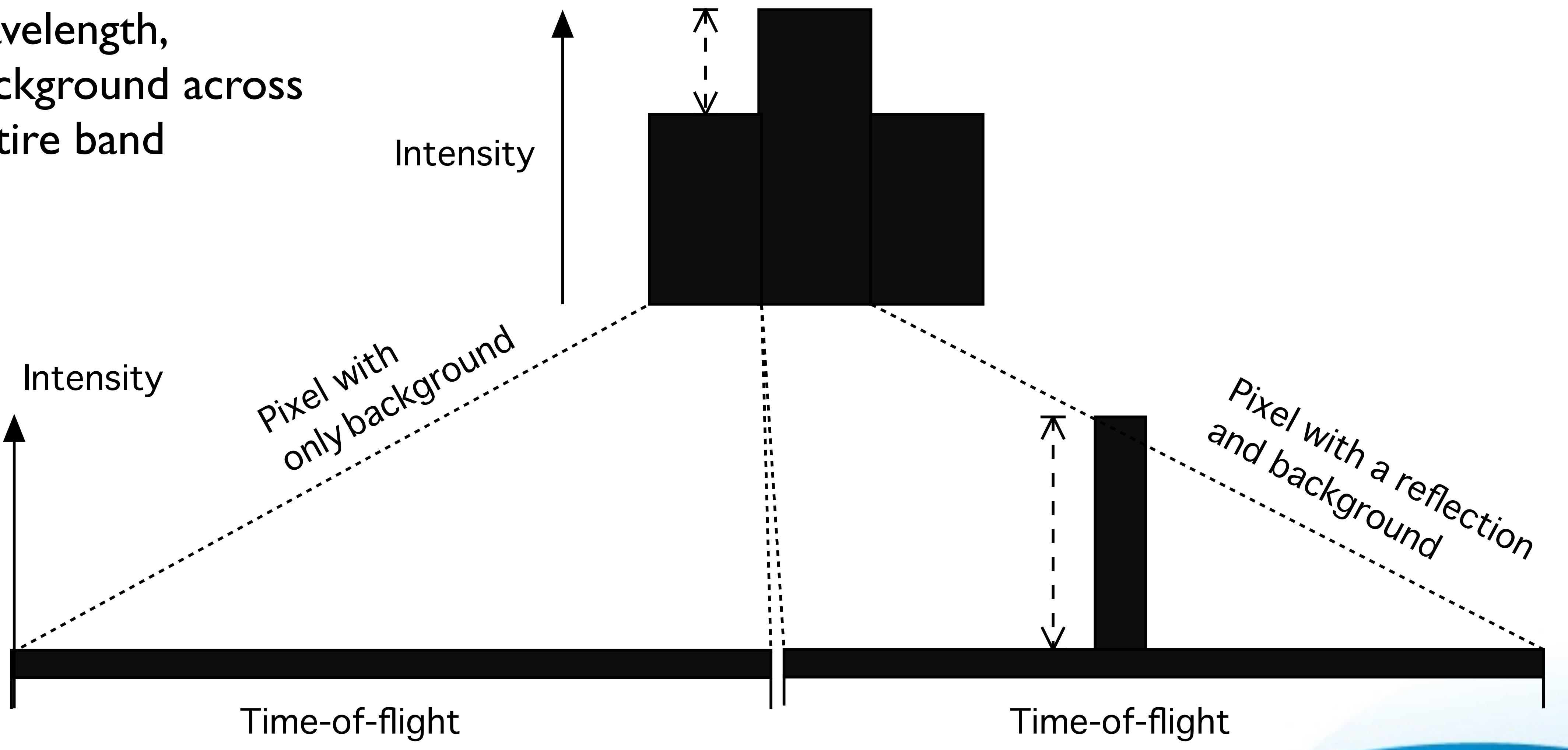
- Solid angle coverage can be traded for unit cell size
- Large unit cells will take longer to collect

Detectors – technological risk and mitigation strategy

- R&D required to reach 0.2 mm spatial resolution with reasonable area and efficiency
- Gd coated gas electron multiplier (GEM) detectors promising – prototypes developed at CERN
- Decision on detector technology is needed late 2016
- ESS Detector Group has prioritised this R&D – collaboration with CERN (2 FTE from autumn 2013)
- Boron coated GEM is a fallback option with compromised efficiency

Spreading background over time-of-flight

Laue method ➔ signal at one wavelength, background across entire band



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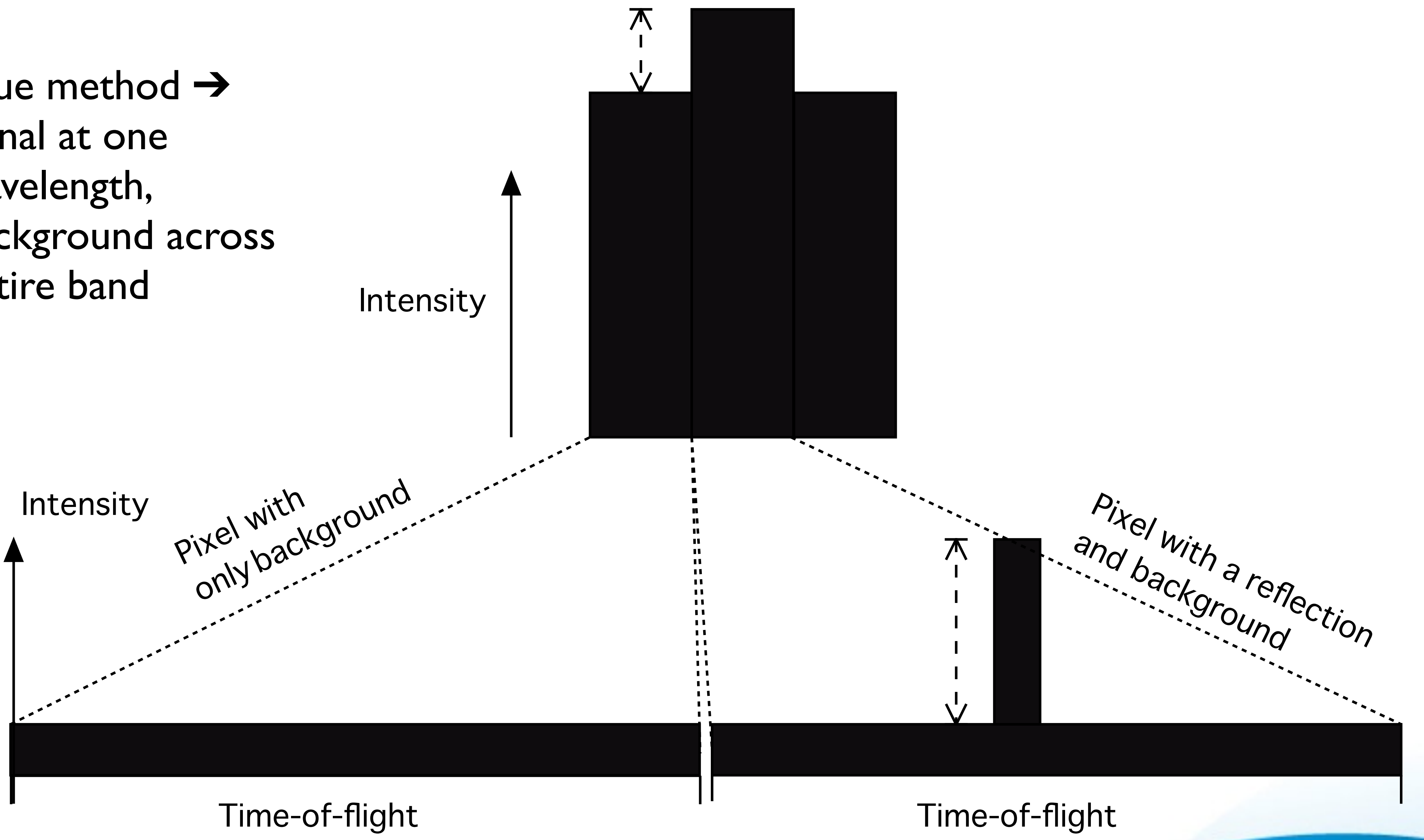

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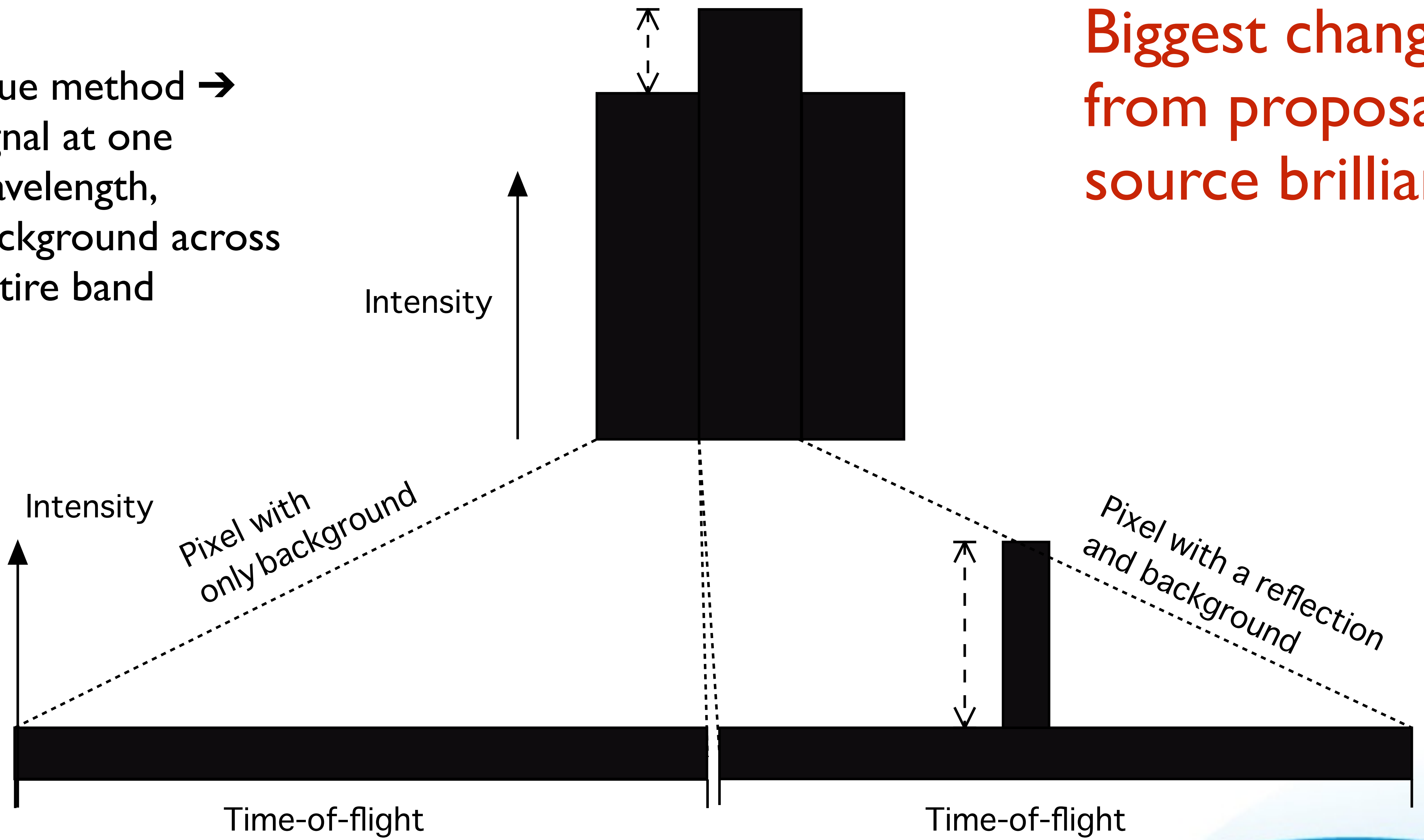

Biggest change from proposal is source brilliance!

Flux at sample – time averaged

- By Monte Carlo simulation 1.8×10^9 n/s/cm^2 at ±0.2° divergence
- By Monte Carlo simulation 9.4×10^8 n/s/cm^2 at ±0.1° divergence
- In proposal analytically 3×10^8 n/s/cm^2 at ±0.1° divergence (simulations agree) — Factor 3
- LADI-III 5×10^7 n/s/cm^2, divergence unclear — Factor 18
- PCS 9.7×10^6 n/s/cm^2 at ±0.1° divergence — Factor 100

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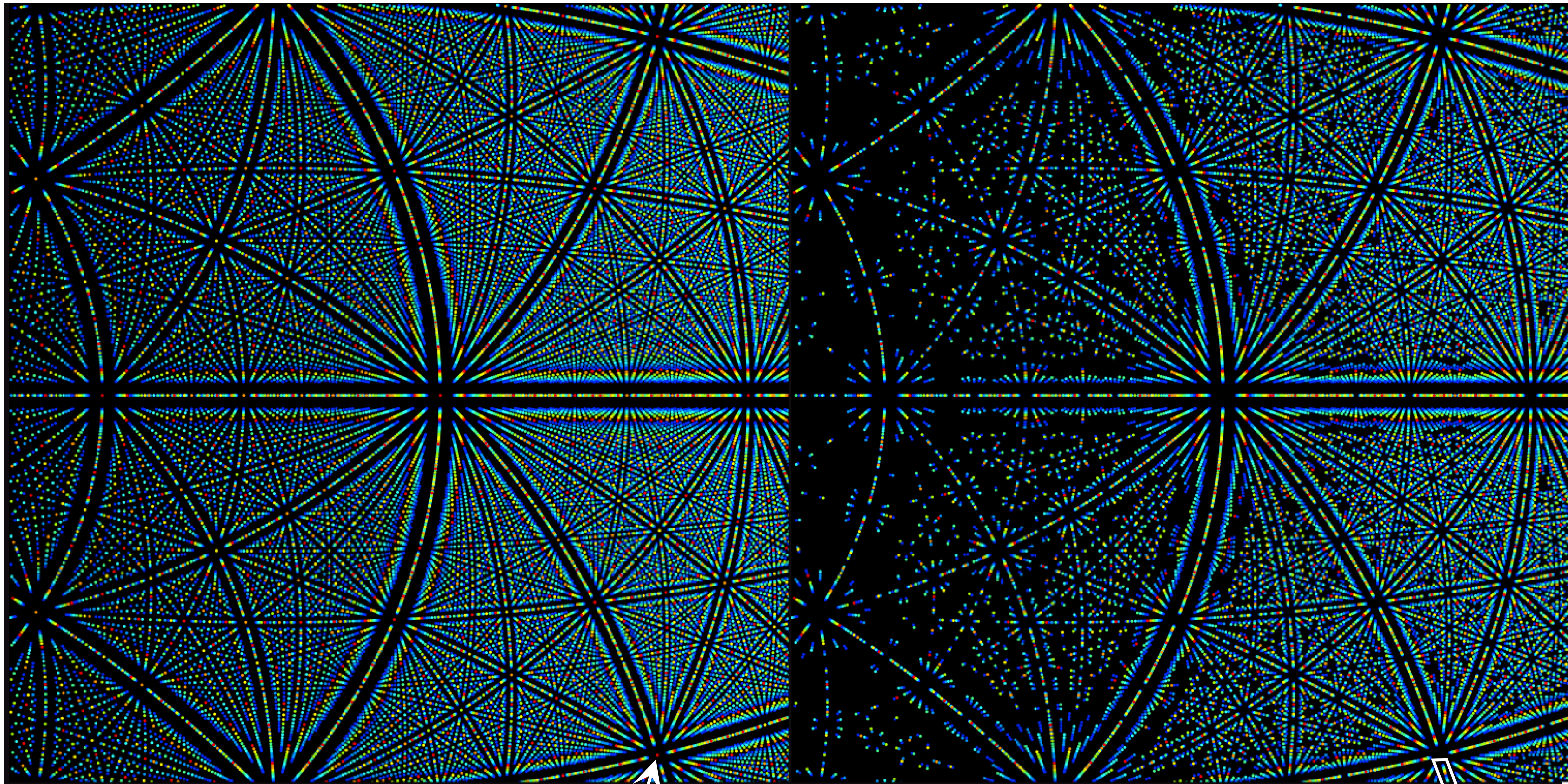
Should be realistic to collect 0.1 mm^3 crystal in < 1 day

Bovine heart cytochrome c oxidase
$P2_12_12_1$
a = 182.59 Å
b = 205.40 Å
c = 178.25 A
Detector distance 1 m



All reflections

14 28 42 (3.409 Å, 134.4 ms) 21 35 49 (2.809 Å, 110.8 ms)
15 29 43 (3.309 Å, 130.5 ms) 22 36 50 (2.739 Å, 108.0 ms)
16 30 44 (3.215 Å, 126.8 ms) 23 37 51 (2.672 Å, 105.4 ms)
17 31 45 (3.124 Å, 123.2 ms) 24 38 52 (2.608 Å, 102.9 ms)
18 32 46 (3.040 Å, 119.9 ms) 25 39 53 (2.548 Å, 100.5 ms)
19 33 47 (2.959 Å, 116.7 ms) 26 40 54 (2.489 Å, 98.2 ms)
20 34 48 (2.882 Å, 113.6 ms)

- 1.800 to 2.019 Angstroms
- 2.019 to 2.237 Angstroms
- 2.237 to 2.456 Angstroms
- 2.456 to 2.675 Angstroms
- 2.675 to 2.894 Angstroms
- 2.894 to 3.112 Angstroms
- 3.112 to 3.331 Angstroms
- 3.331 to 3.550 Angstroms

Spatial overlaps only

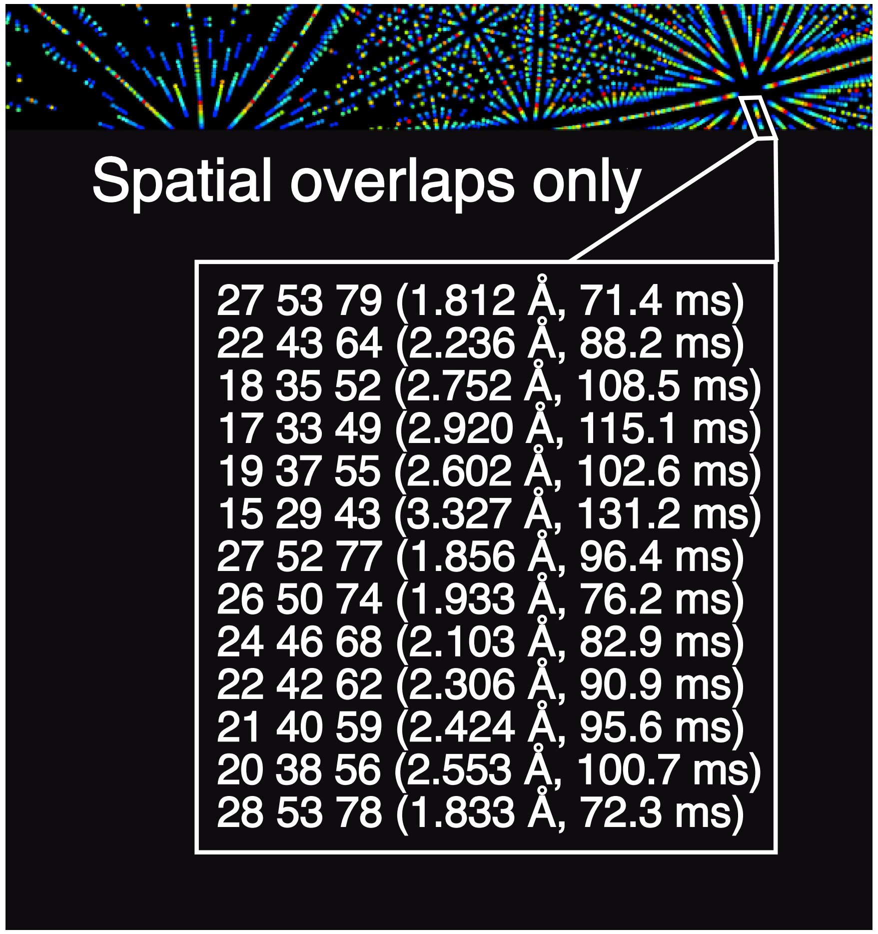
27 53 79 (1.812 Å, 71.4 ms)
22 43 64 (2.236 Å, 88.2 ms)
18 35 52 (2.752 Å, 108.5 ms)
17 33 49 (2.920 Å, 115.1 ms)
19 37 55 (2.602 Å, 102.6 ms)
15 29 43 (3.327 Å, 131.2 ms)
27 52 77 (1.856 Å, 96.4 ms)
26 50 74 (1.933 Å, 76.2 ms)
24 46 68 (2.103 Å, 82.9 ms)
22 42 62 (2.306 Å, 90.9 ms)
21 40 59 (2.424 Å, 95.6 ms)
20 38 56 (2.553 Å, 100.7 ms)
28 53 78 (1.833 Å, 72.3 ms)

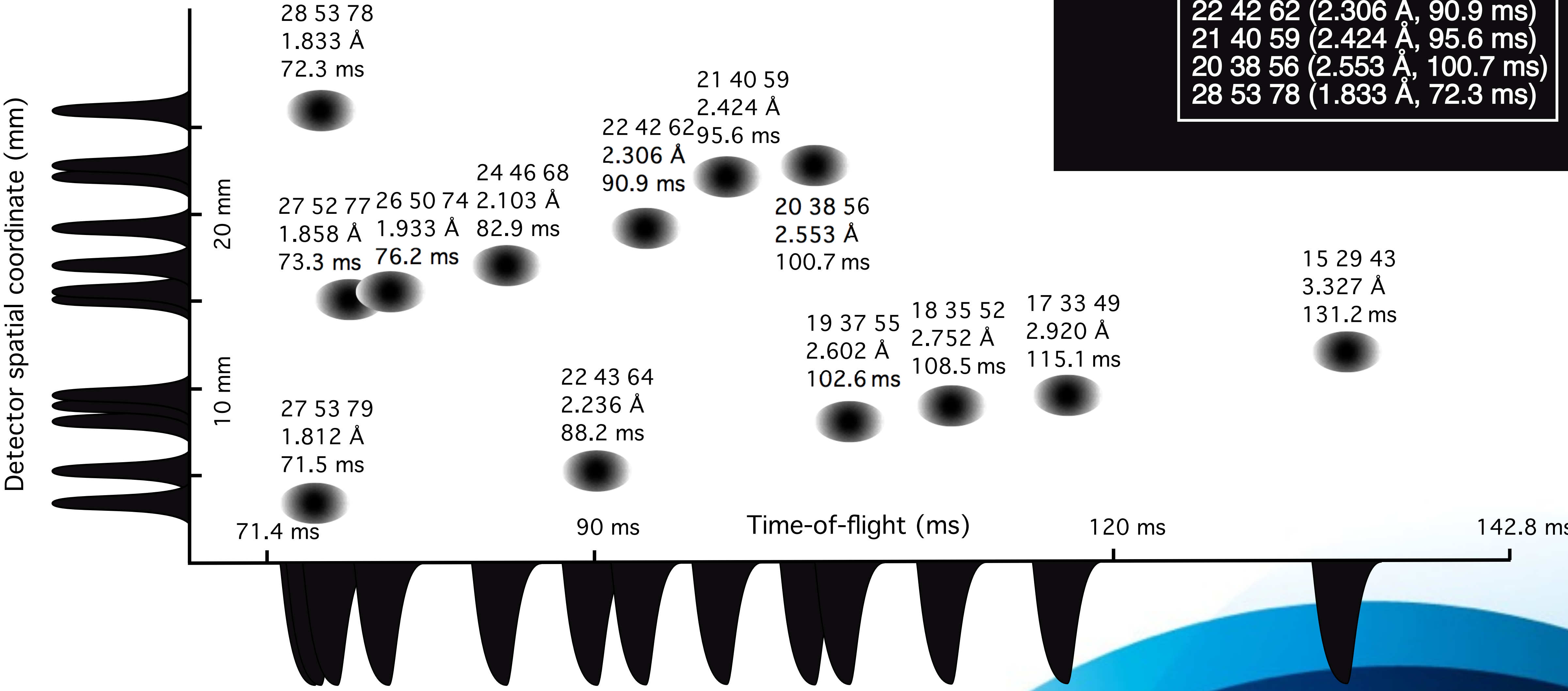
Generated using the Daresbury Laue Suite

Campbell et al. J. Appl. Cryst. (1998). 31, 496-502
Artz et al. J. Appl. Cryst. (1999). 32, 554-562
Helliwell, J.R. et al. J. Appl. Cryst. (1989) 22, 483–497

Overlap separation with TOF

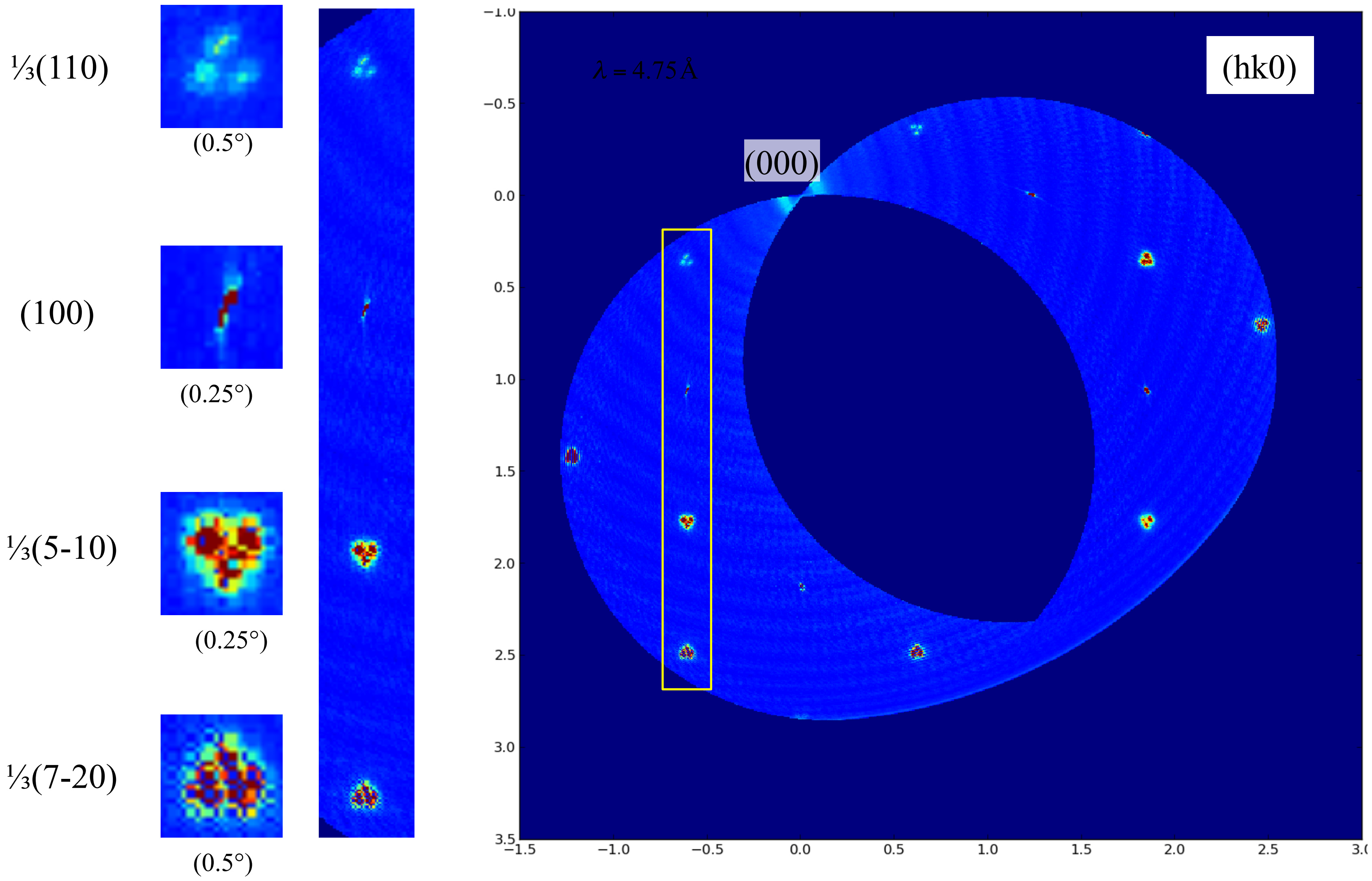
Bovine heart cytochrome c oxidase
$P2_12_12_1$
a = 182.59 Å
b = 205.40 Å
c = 178.25 A
Detector distance 1 m





Magnetic crystallography at a macromolecular diffractometer

BioDiff, FRM-2, Munich



λ= 4.75 Å

Johannes Reim, Werner Schweika (FZJ, ESS), Andreas Ostermann, Tobias Schrader (TUM)

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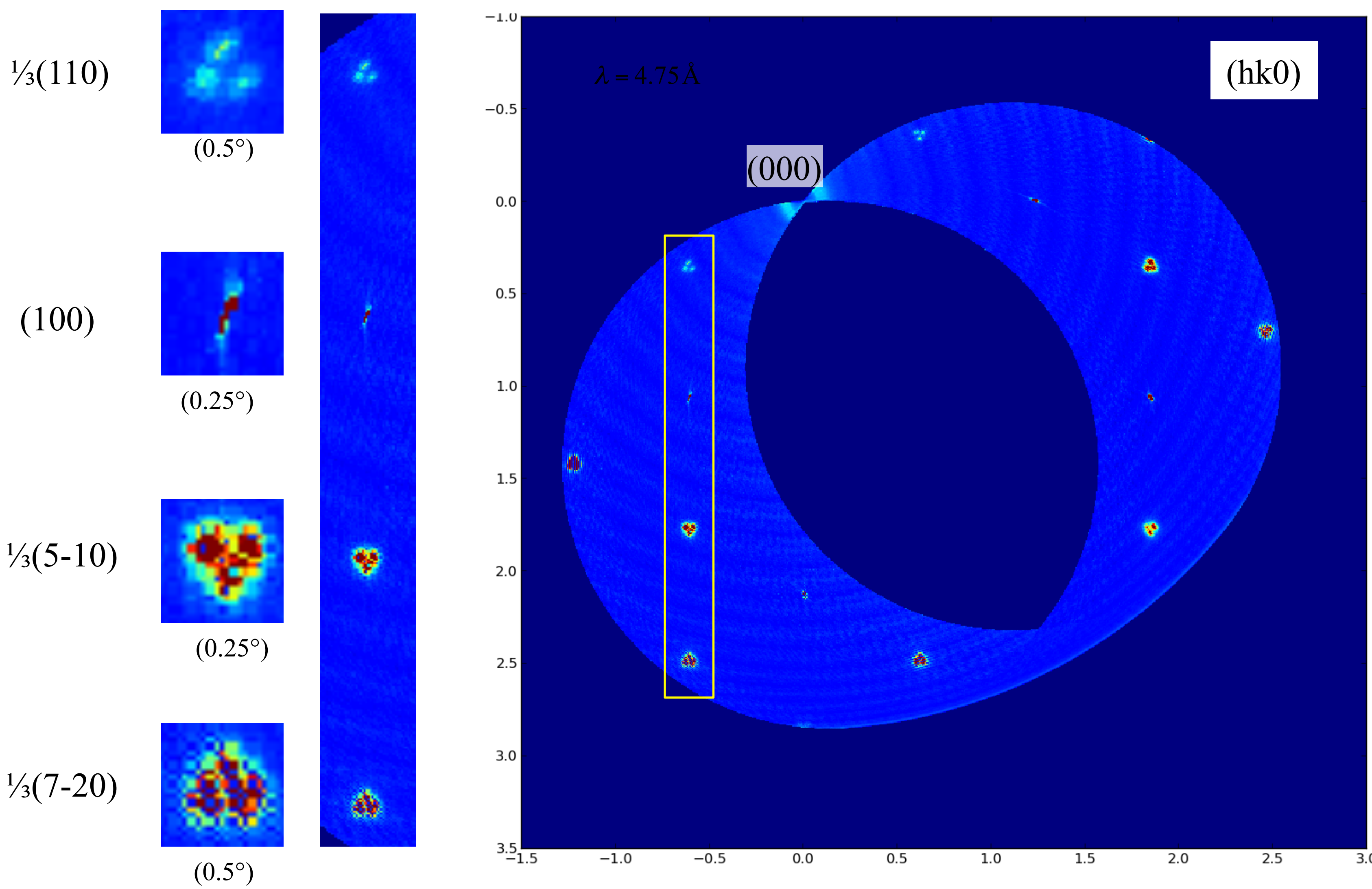

With NMX integrated intensities can be obtained with a single orientation without sacrificing q-resolution

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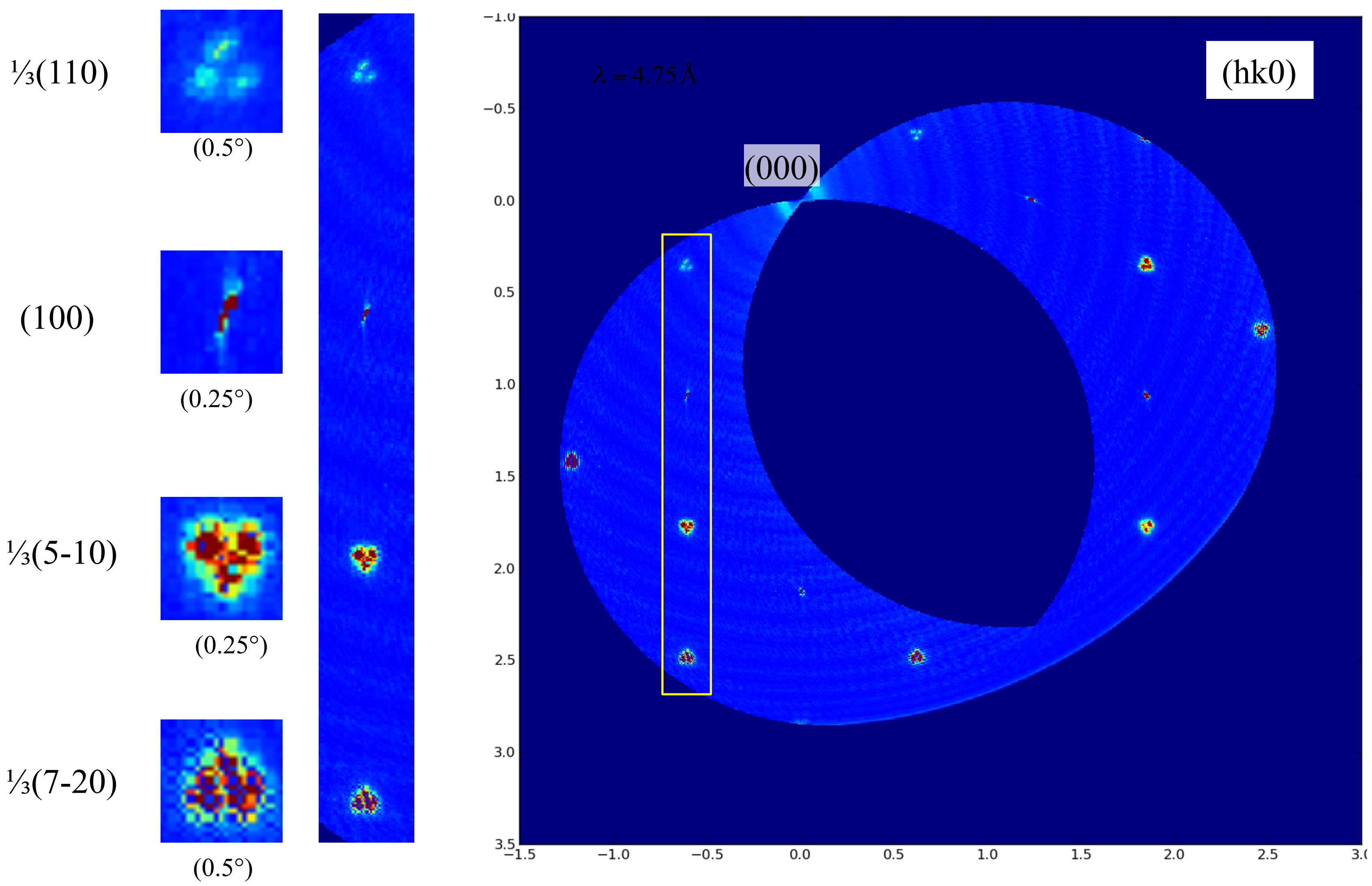


With NMX integrated intensities can be obtained with a single orientation without sacrificing q-resolution

Data collection > 300 times faster!

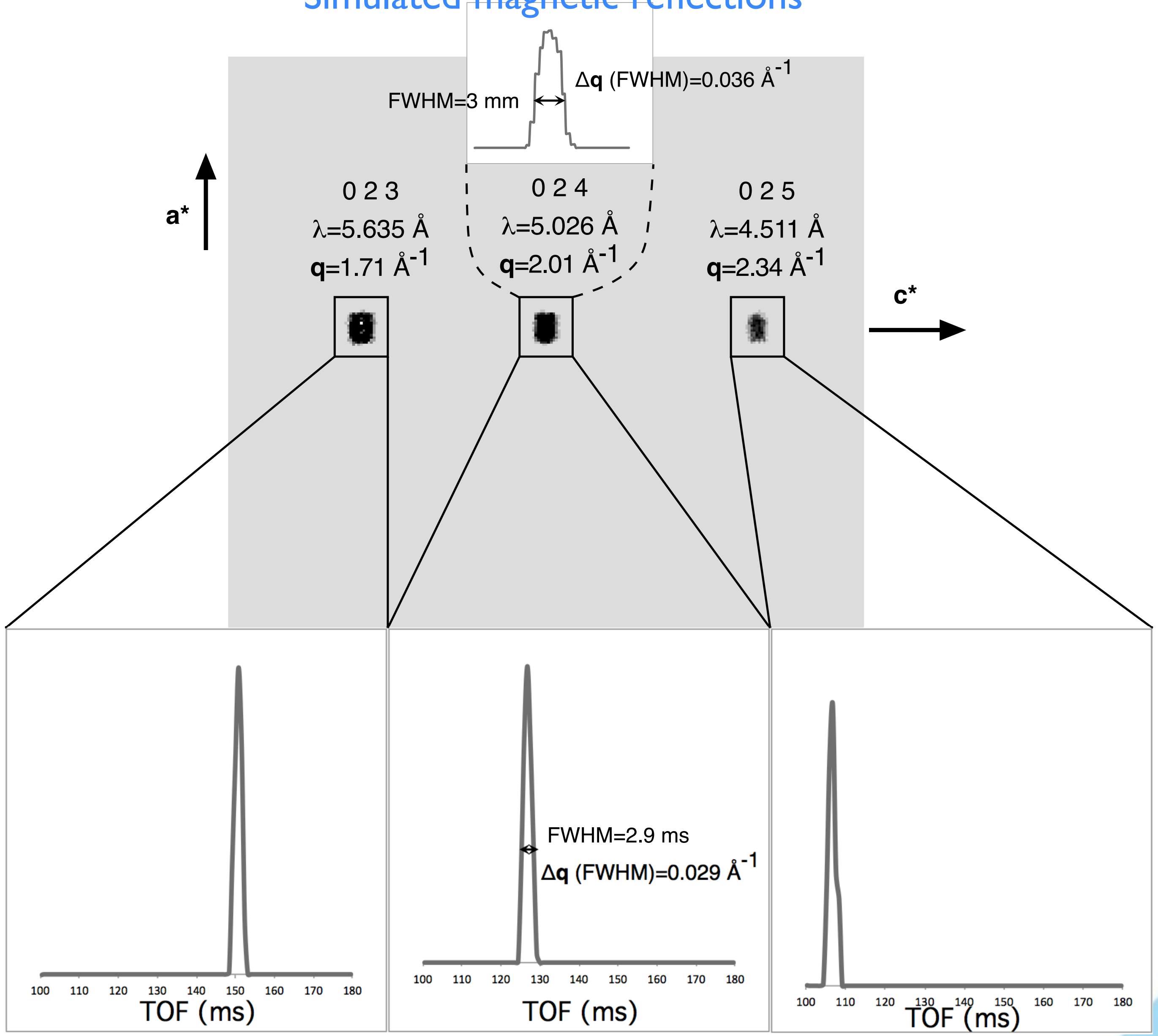
λ= 4.75 Å

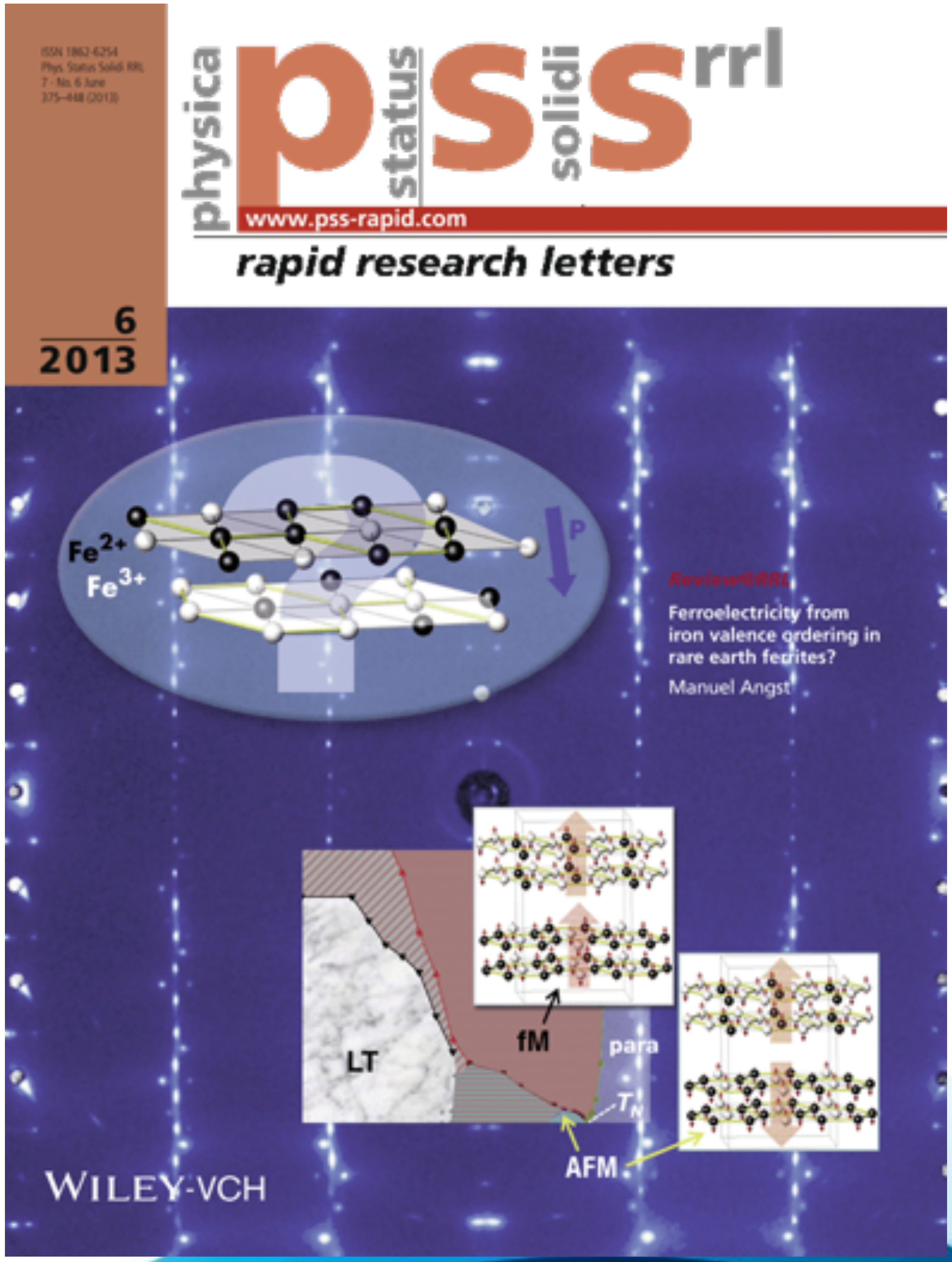
Johannes Reim, Werner Schweika (FZJ, ESS), Andreas Ostermann, Tobias Schrader (TUM)

Magnetic structures at ESS NMX

- Magnetic ordering in a proposed charge-ordered ferroelectric ($LuFe_2O_4$)
- Magnetic superstructure peaks easily integrateable
- **q**-resolution allows peak splitting to be observed

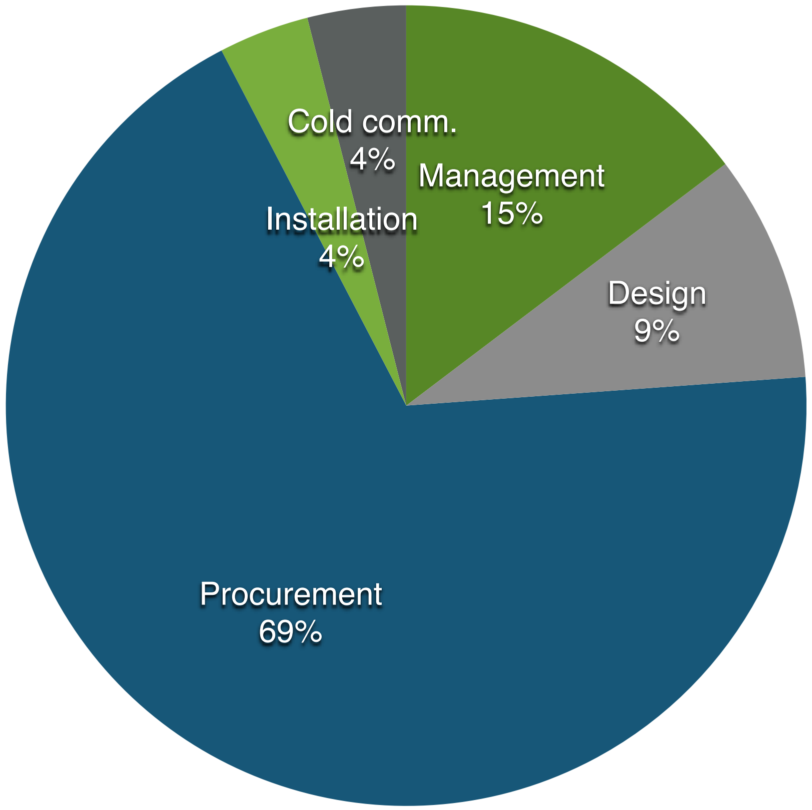
Simulated magnetic reflections



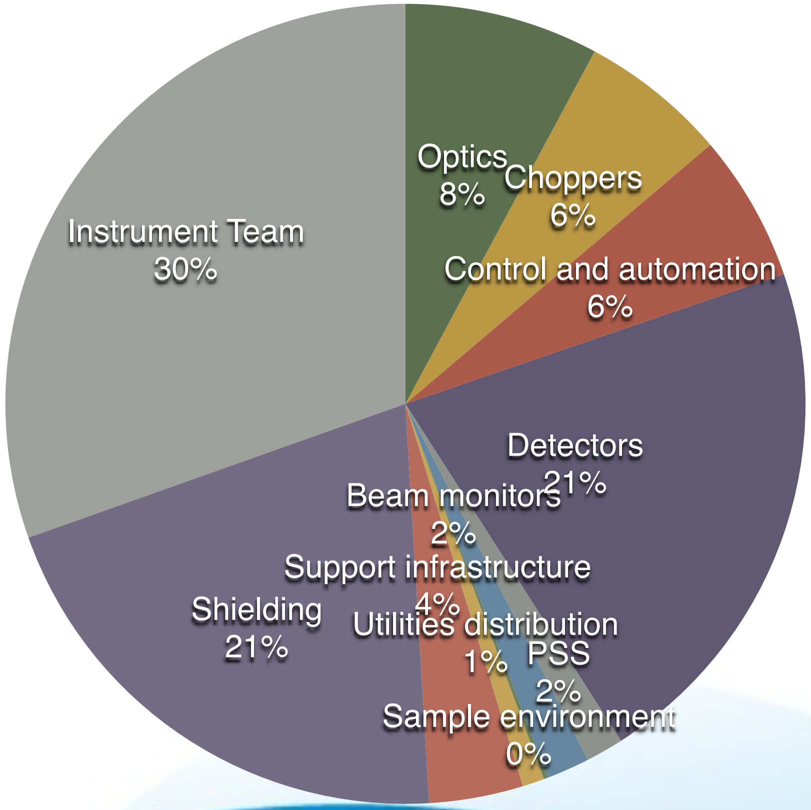


Manuel Angst (FZJ)

Budget overview



Work Unit	Management	Design	Procurement	Installation	Cold commissi oning	Total
Instrument Team	1 150 560 €	633 120 €	4 224 541 €	352 229 €	88 800 €	**6 449 250 €**
Neutron Optics and Shielding Group	0 €	0 €	909 000 €	0 €	0 €	**909 000 €**
Neutron Chopper Group	74 360 €	53 920 €	517 280 €	30 560 €	13 560 €	**689 680 €**
Neutron Detector Group	126 750 €	243 000 €	2 012 200 €	0 €	276 600 €	**2 658 550 €**
Sample Environment Team	5 760 €	4 320 €	5 760 €	2 400 €	2 400 €	**20 640 €**
Motion Control and Automation	59 400 €	66 720 €	144 220 €	5 040 €	56 880 €	**332 260 €**
Personnel Safety System	3 080 €	53 760 €	70 000 €	30 720 €	19 200 €	**176 760 €**
Phase 1	270 000 €					**270 000 €**
Total	**1 689 910 €**	**1 054 840 €**	**7 883 001 €**	**420 949 €**	**457 440 €**	**11 506 140 €**



Non labour	Labour
6 853 041 €	4 653 099 €

Manuel Angst (FZJ)

NMX staging plan – based on Cost Category letter

- NMX was assigned Cost Category B (12 M€)
- Cost estimate 11 506 140 €
- Staging plan becomes upgrade plan
- Upgrade 1 (to Cost Category limit): Enriched Gd coating, efficiency increase from 20% to 35 %, cost estimate 300 k € –1 M€
- Upgrade 2 (beyond Cost Category limit): 3 more detectors, doubles throughput, cost estimate (very rough) 1,8 M€

Note
Document Number ESS-00179[illegible]
Date Wednesday, 12 November 2014

To: Esko Oksanen and Guiseppe Aprigliano

Subject: Provisional Cost Category for *NMX* Instrument Project

The ESS project welcomes the inclusion of the *NMX* concept into the NSS Instruments baseline after advice from the SAC and approval from our Steering Committee.

The *NMX* instrument team or consortium is authorised to commence work towards completion of the "Phase 1 – Preliminary Engineering Design" from January 2013 onwards.

During "Phase 1 – Preliminary Engineering Design" a detailed plan, schedule and cost is to be developed as described in "Process for Instrument Design and Construction".

ESS management has reviewed the initial costing of the *NMX* Instrument Project as described in the instrument proposal. On this basis we assigned *Cost Category B* as indicated in [1], which defines an upper cost limit (baseline + contingency) of 12 Mio€$_{Net}$ for this instrument project.

Instruments projects in Phase 1 are to work towards a validation of this cost category and provide project plans for (i) a functional instrument while retaining a 10% internal contingency within their cost category, (ii) a plan of how the internal contingency could be used towards achieving the full scope of the instrument and (iii) a staging plan that achieves an enhanced scope of the instrument utilising finances outside of the cost category.

ESS will be taking responsibility for certain work packages or work units that are within the cost category. These are described in Appendix 1.

In addition to the budget described by this cost category, ESS will contribute to the instrument 2.7 Mio€ of scope value described in the Appendix 1.

We wish you every success in realising *NMX.*

D. N. Argyriou
NSS Project Director

Distribution list
Ken Andersen, Robert Connatser and Oliver Kirstein

References
[1] ESS Construction Phase Cost Book 2014

NMX cost risks and mitigation – descoping

Risk	Probability	Consequence	Mitigation	Comments
Detector cost estimates are exceeded	2	2	Use of contingency, descoping	
Shielding thickness increases after neutronics calculations	2	2	Use of contingency, descoping detectors	In the case of a large cost increase in shielding, NSS contingency may be released
Optics cost increases	1	2	Use of contingency, descoping detectors	

NMX cost risks and mitigation – descoping

Risk	Probability	Consequence	Mitigation	Comments
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NMX scope contingency

Item	Scope reduction	Cost impact	Scientific impact	Comments
Detector unit	Not procure	343 k€/unit	increased data collection time	Per unit cost increases ~100% if procured one by one
Sample environment	Not procure	67 k€	Some experiments become impossible	Short lead time in procurement
Chopper 2 2nd disc	Leave out	60 k€	Cannot tailor bandwidth	Not readily recoverable

Questions?