DRAC or DRACULA ?

Diffractometer for
Rapid
ACquisition

DRAC, a water dragon (*Draco)* living at the mouth of the Rhone

DRAC or DRACULA ?

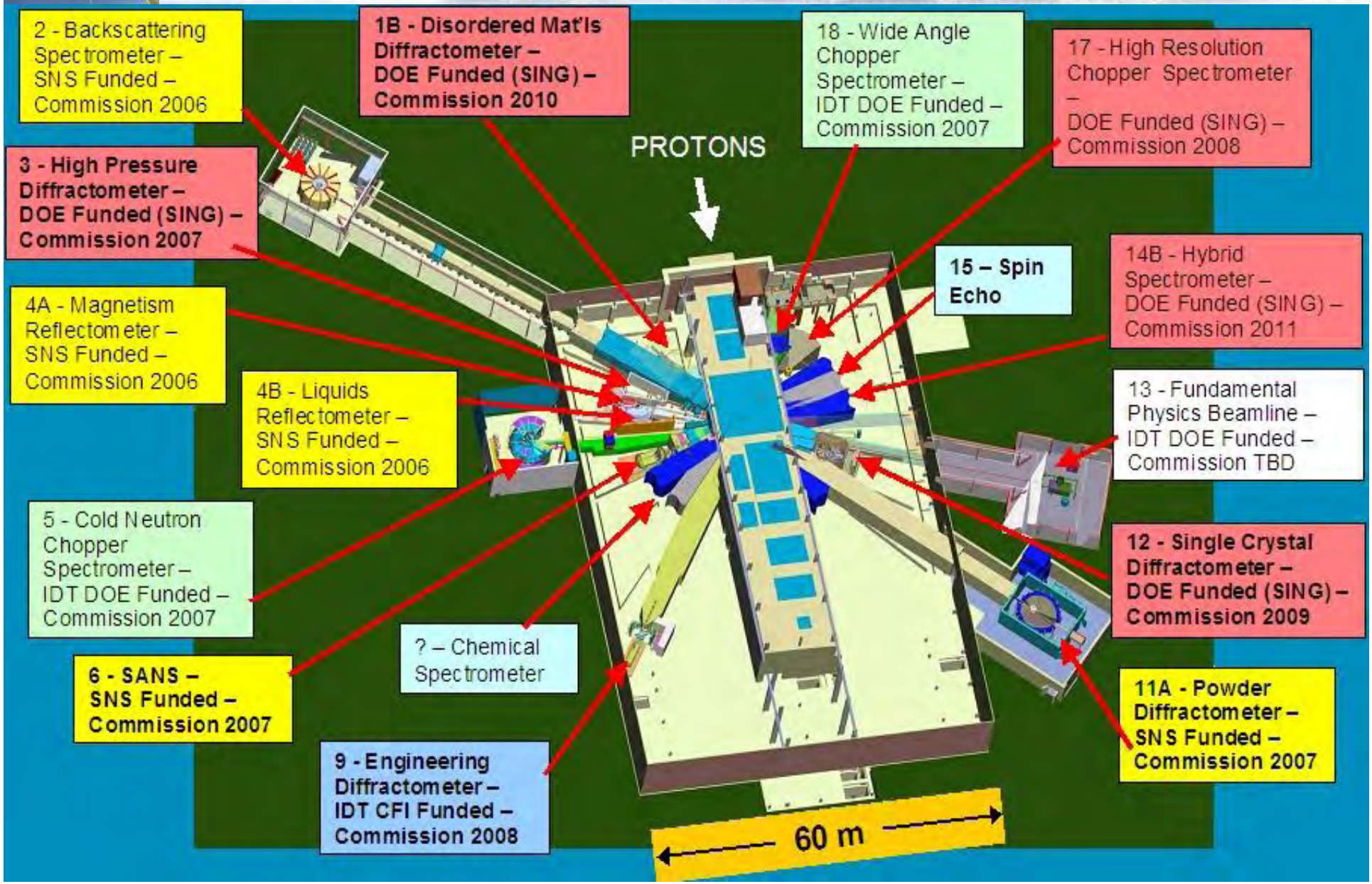
Diffractometer for
Rapid
ACquisition
Ultra
Large
Areas

DRAC, first presented at ILL "Instrument Day" 26 Feb 2002

DRAC, highest priority for Instrument Committee 17 Oct 2003

Hypnotised by the American SNS ?

Instruments on the American SNS



POW-GEN3 Powder Diffractometer at SNS

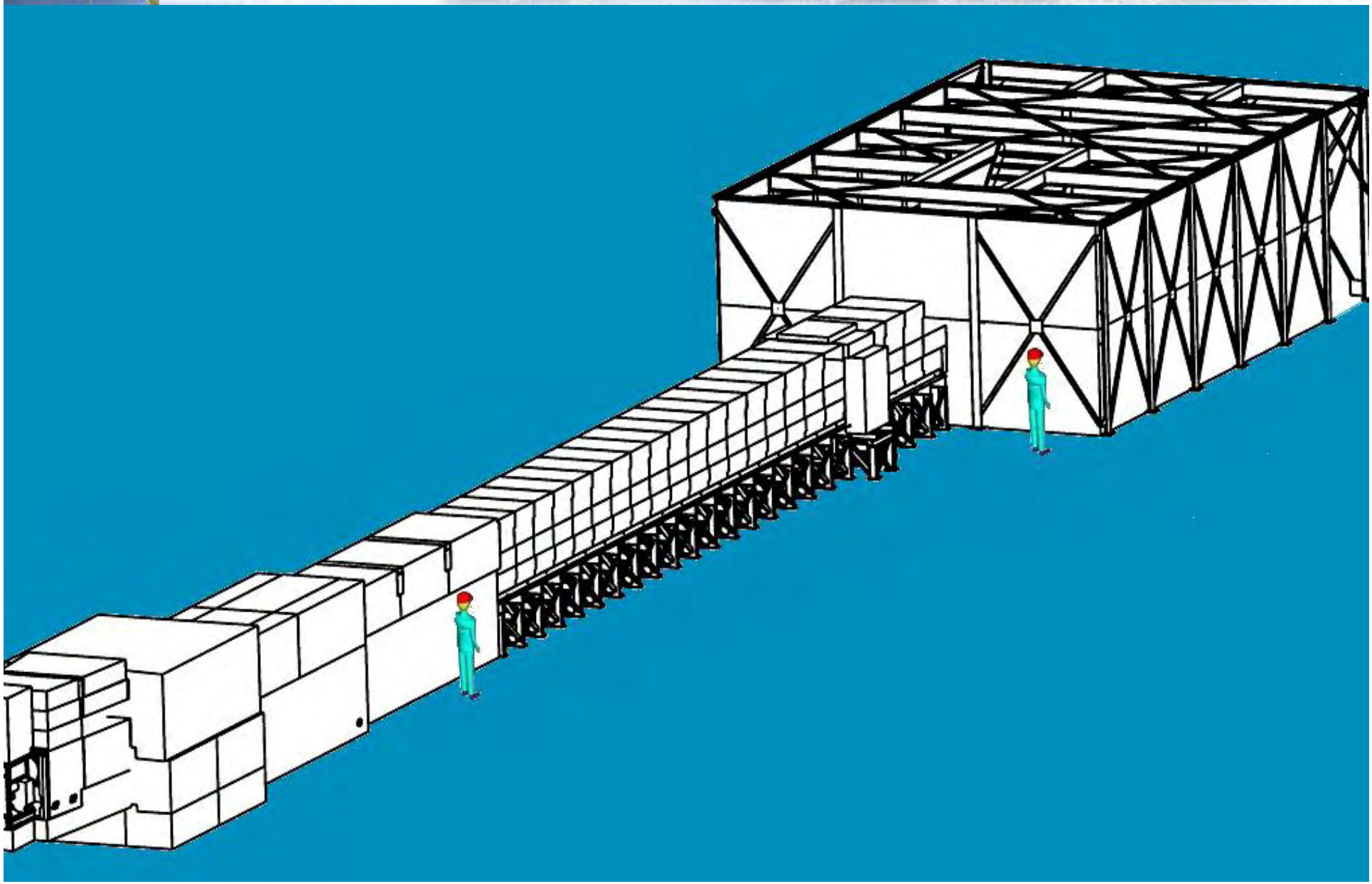
SNS-EFAC recommendations

- "…the SNS should immediately begin work on the conceptual design for… a third generation powder diffractometer with a resolution $\Delta d/d$ of ~1×10^{-3} at 90°." Nov 1998.

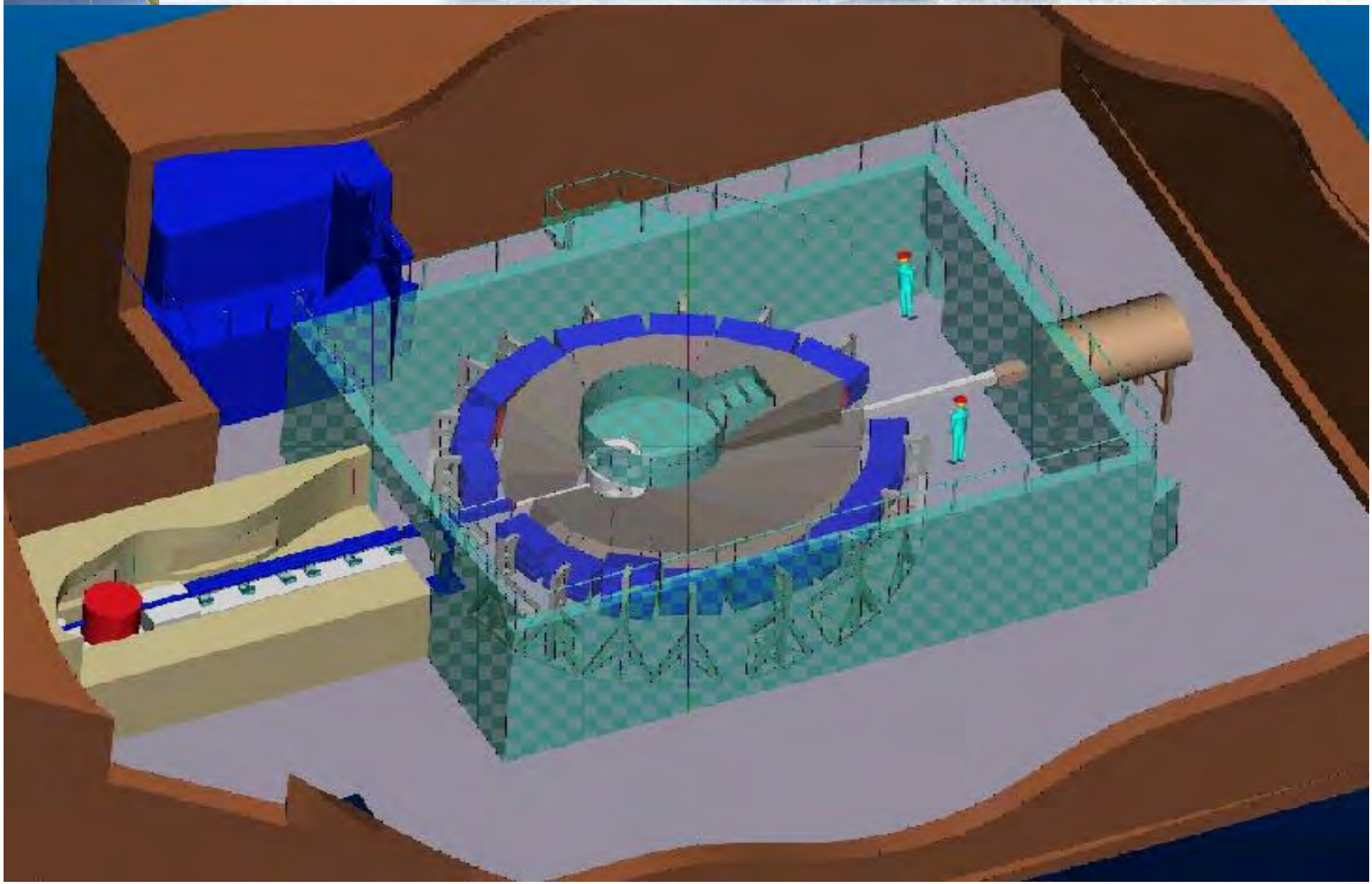
Note: Moderately high resolution at 90° scattering.

- "SNS without a world-class powder diffractometer on day one is unthinkable." May 2001.
- "1.1 Recommendation: A high level of priority should be assigned to bringing the powder diffractometer (POW-GEN3) into operation as early as possible." Dec 2003.

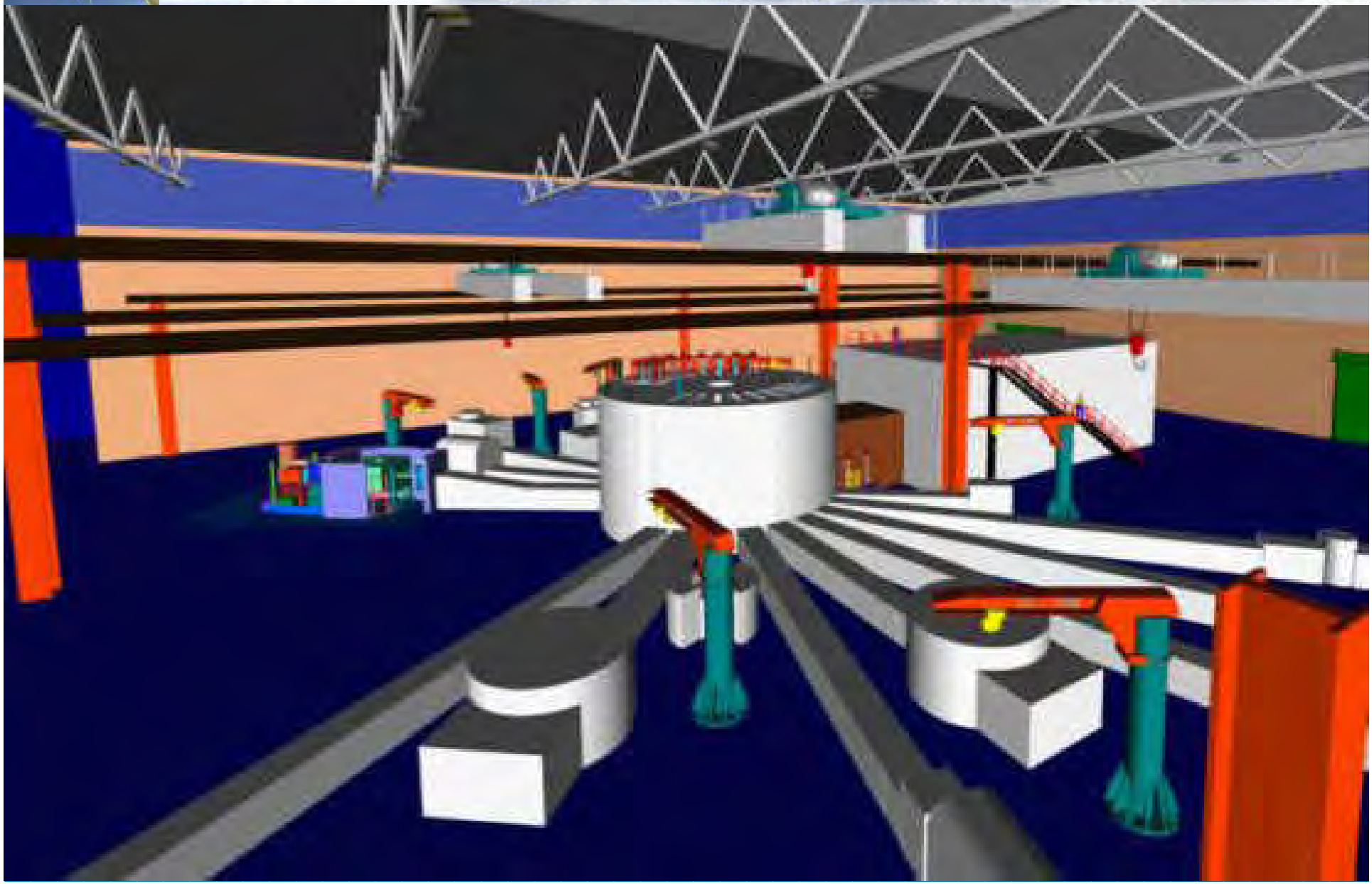
POW-GEN3 at SNS – a BIG detector



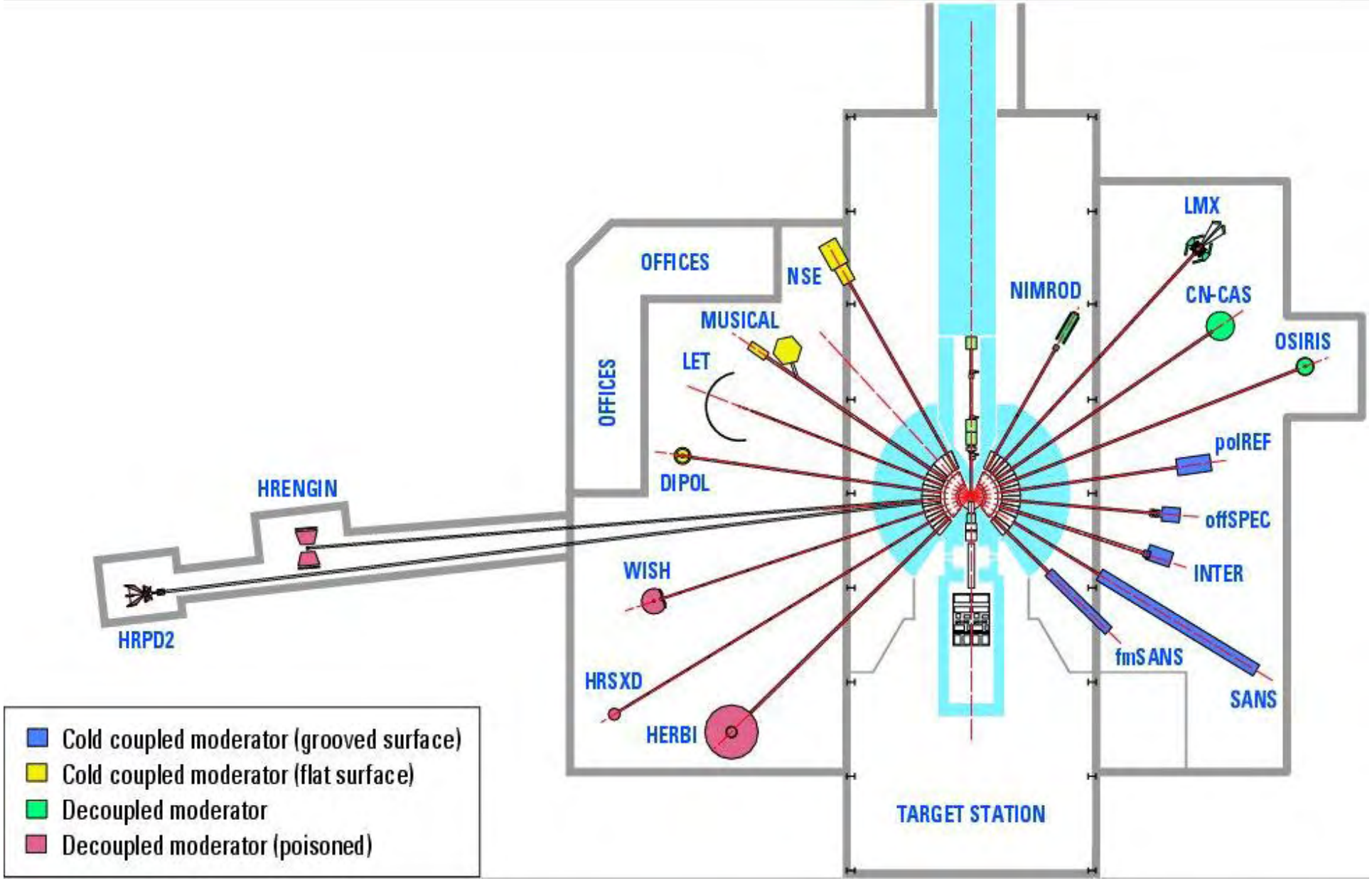
POW-GEN3 at SNS – a BIG detector



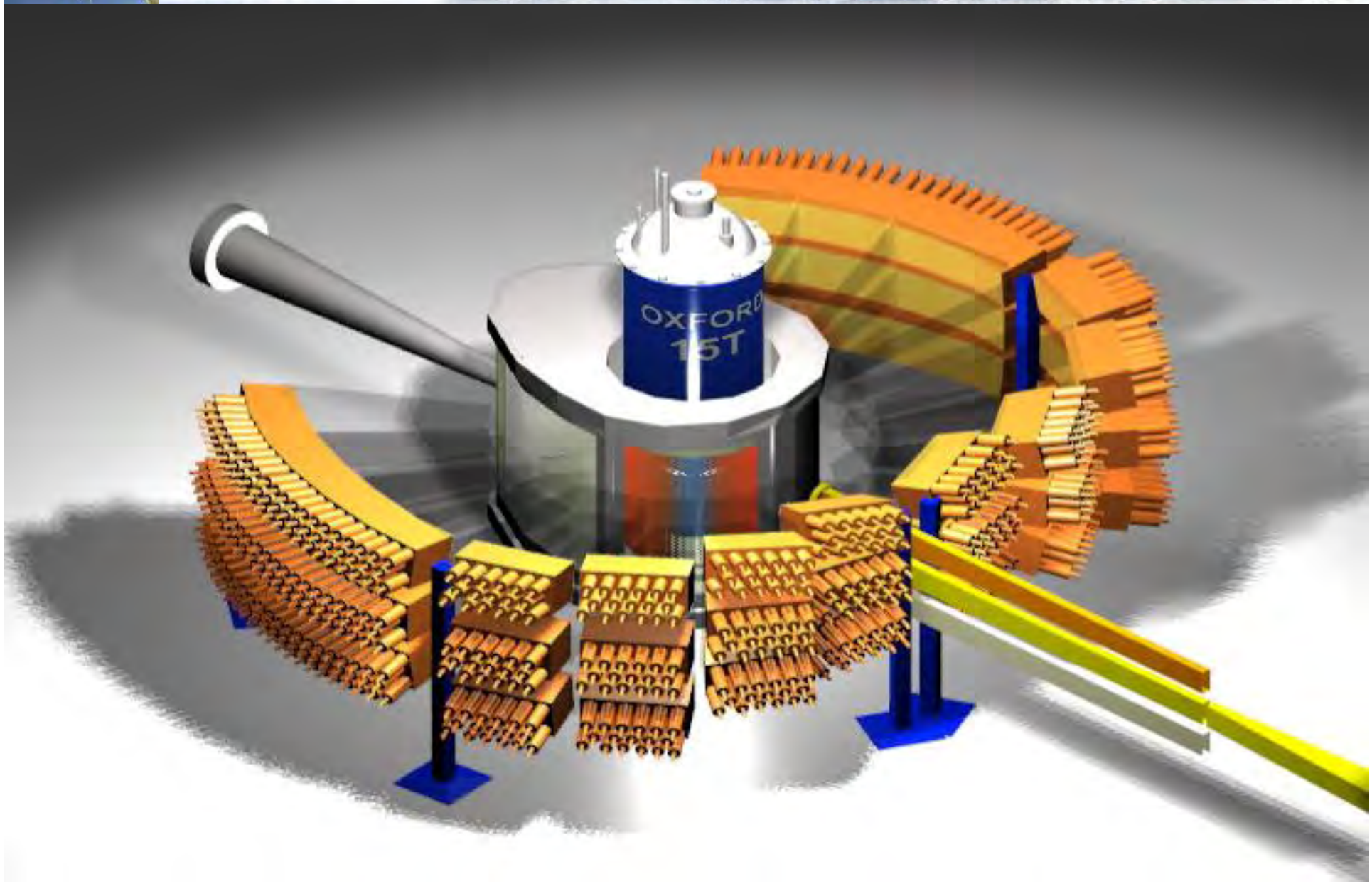
Target Station-2 at ISIS



Target Station-2 at ISIS



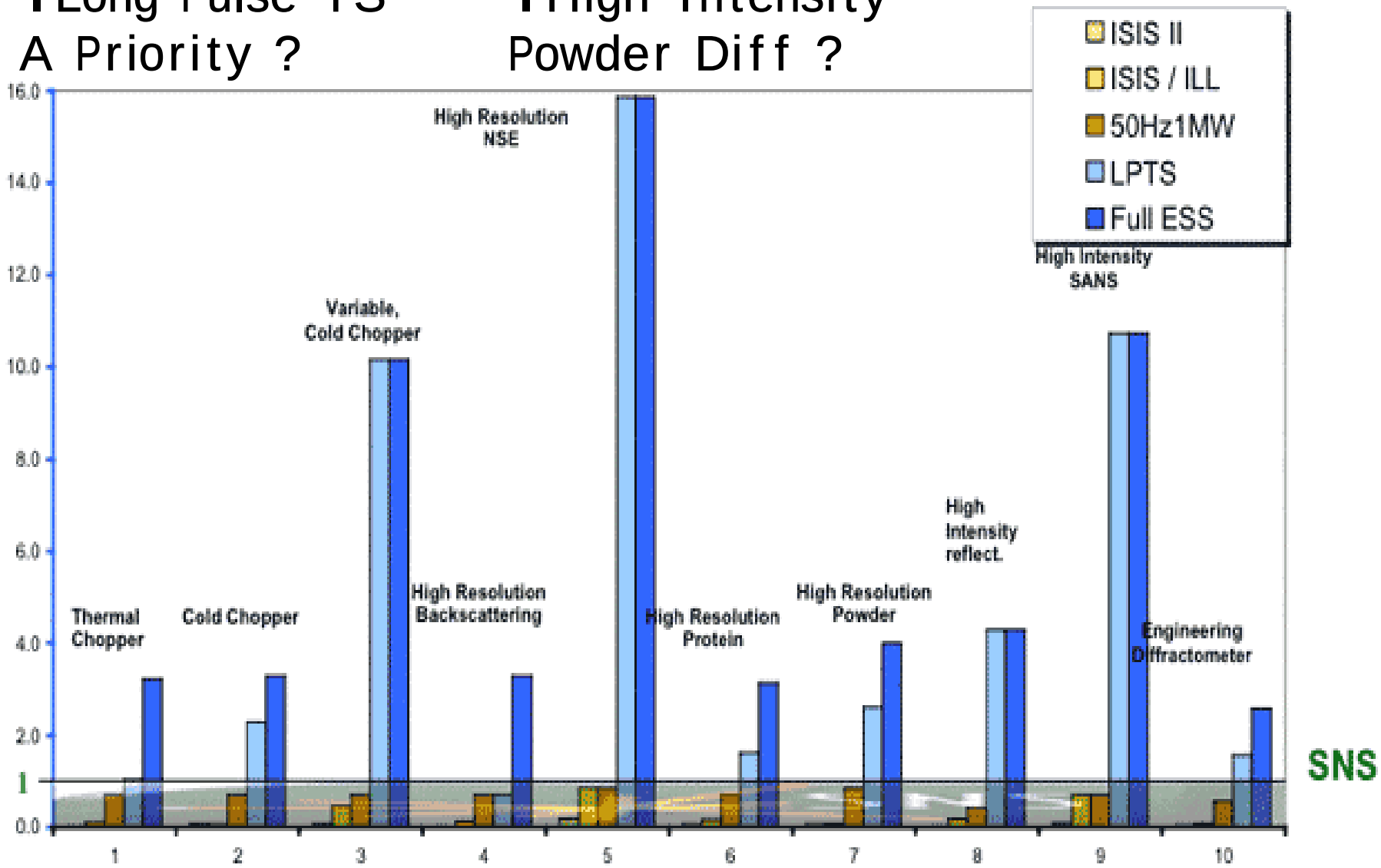
WISH Powder Diffractometer, TS2-ISIS



While we are waiting for the ESS dream…

While we are waiting for the ESS dream…

- Long Pulse TS A Priority ?
- High Intensity Powder Diff ?



SNS

Proposed ESS Powder Diffractometers

- ST05 High-Q Powder Diffractometer HQP
- ST06 Liquids & Amorphous Diffractometer LAD
- SM10 Single Pulse Diffractometer SPD
- SD17 Magnetic Powder Diffractometer MagP
- SD18 High Resolution Powder Diffractometer HRPD
- LM05 Ultra-high Resolution Powder Diffractometer URPD
- LM06 High Pressure Powder Diffractometer HiPD

Powder Diffractometer Efficiency

ESS Instrumentation Group Reports, May 2001

Powder Diffraction Instruments

P.G. Radaelli, S. Hull , H.J. Bleif & A. M. Balagurov

- Given the choice, the 50Hz target is always better than the 10Hz one.
- We dearly miss a truly sharp cold moderator, especially for crystallography requiring high and low Q at the same time.
- The 50Hz target would be the first choice for all powder (and probably single-crystal) diffractometers.

Powder Diffractometer Efficiency

ESS Instrumentation Group Reports, May 2001

Powder Diffraction Instruments

P.G. Radaelli, S. Hull , H.J. Bleif & A. M. Balagurov

The average count rate is the product of:

- the flux at the sample
- the detector solid angle and efficiency
- the sample volume

Powder Diffractometer Efficiency

ESS Instrumentation Group Reports, May 2001

Powder Diffraction Instruments

P.G. Radaelli, S. Hull , H.J. Bleif & A. M. Balagurov

- Reactor-based instruments tend to maximise the source solid angle, by exploiting focusing monochromators (flux)
- Diffractometers at pulsed sources tend to have much larger detector solid angles.

Powder Diffractometer Efficiency

ESS Instrumentation Group Reports, May 2001

Powder Diffraction Instruments

P.G. Radaelli, S. Hull , H.J. Bleif & A. M. Balagurov

Conclusions:

- TOF machines need a higher flux source (SNS,ESS)
- CW machines need a larger detector (which is somewhat less expensive).

Comparison of TOF & CW Diffractometers

Jorgensen, J.D., Cox, D.E., Hewat, A.W., Yelon, W.B (1984)

"Scientific opportunities with advanced facilities for neutron scattering"

Shelter Island Workshop, 1984

Nuclear Instruments and Methods in Physics Research B12 (1985) 525-561

Efficiency for a given resolution = time averaged flux on sample
* sample volume
* detector solid angle

Comparison of TOF & CW Diffractometers

The time-averaged Flux*Detector criterium

D20 has high flux, GEM has a big detector

	D20	GEM
time averaged sample flux	$5x10^7$	$\sim 2x10^6$
detector solid angle	0.27 sr	4.0 sr
efficiency	1.7	1

Comparison of TOF & CW Diffractometers

The time-averaged Flux*Detector criterium

So, let's use a big detector too !

	D20	GEM	DRACULA
time averaged sample flux	5×10^7	$\sim 2 \times 10^6$	$\sim 10^8$
detector solid angle	0.27 sr	4.0 sr	1.5 sr*
efficiency	1.7	1	18

* Based on new D19 detector: R=760 mm, h=400 mm, 800 linear resistive wires 30°x160°

Comparison of TOF & CW Diffractometers

The time-averaged Flux*Detector criterium

Only then can we compete with the SNS.

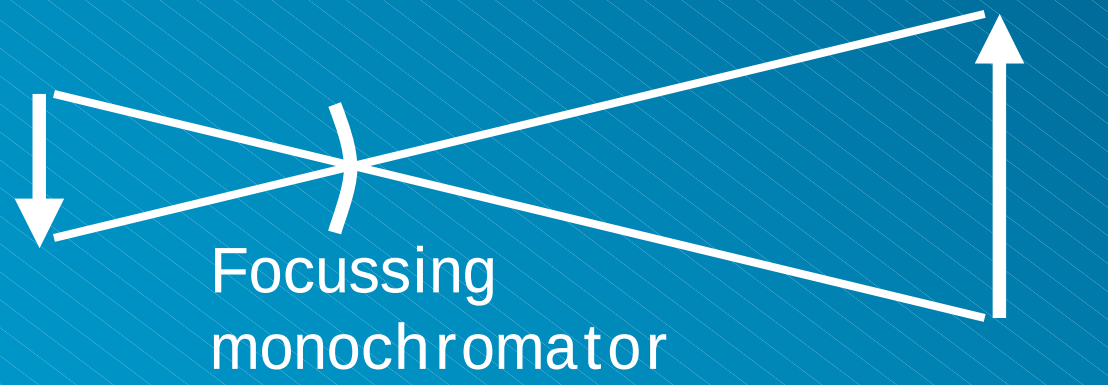
	D20	GEM	DRACULA	SNS
time averaged sample flux	$5x10^7$	$\sim 2x10^6$	$\sim 10^8$	$\sim 2.5x10^7$
detector solid angle	0.27 sr	4.0 sr	1.5 sr*	3.0 sr
efficiency	1.7	1	18	9

* Based on new D19 detector: R=760 mm, h=400 mm, 800 linear resistive wires $30^o x 160^o$

Why is sample flux so high from a reactor?

A: Large vertically focusing monochromators ?

No ! Focusing in real space only
gives a factor of x2 or x3

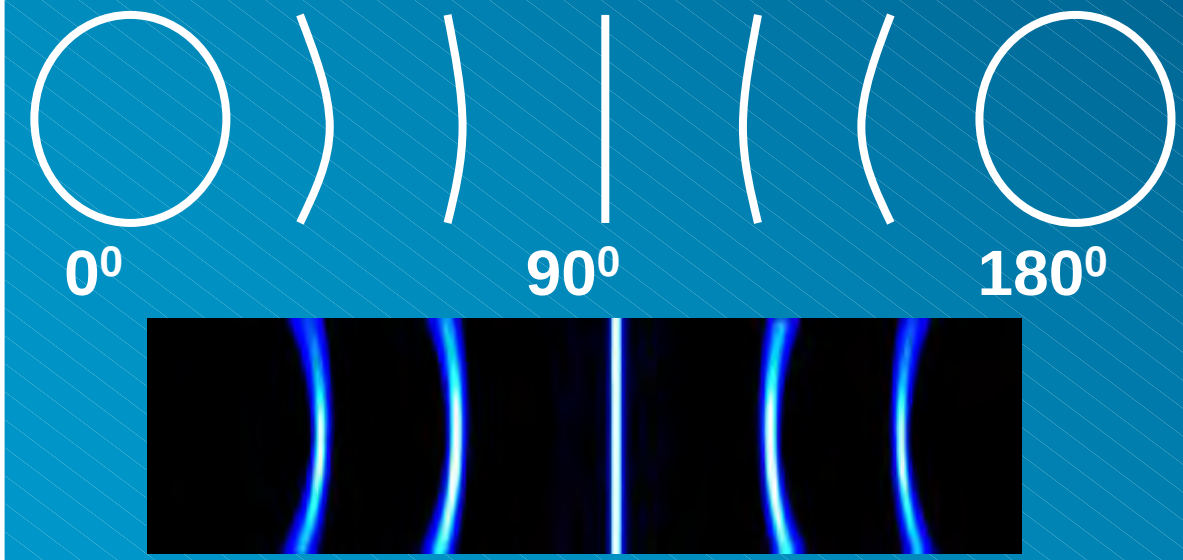


cf use of convergent guide with TOF

Why is sample flux so high from a reactor?

A: Large vertically focusing monochromators ?

Slight smearing of diffraction cones due to monochromator vertical divergence (esp. at very low and very high angles).

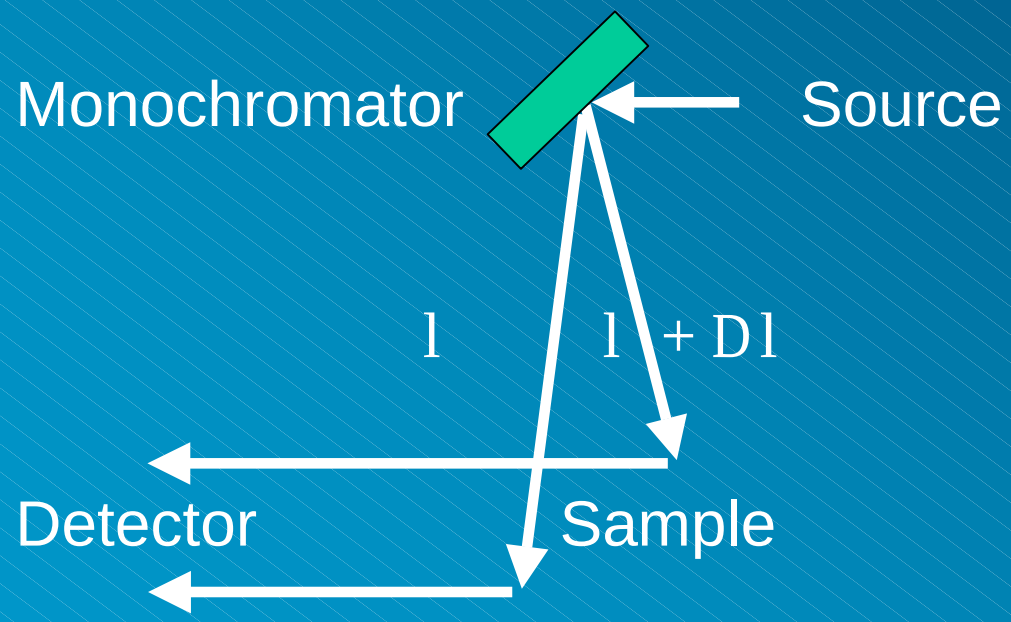


Not a big problem for medium resolution

Why is sample flux so high from a reactor?

A: Large wavelength-band focusing monochromators ?

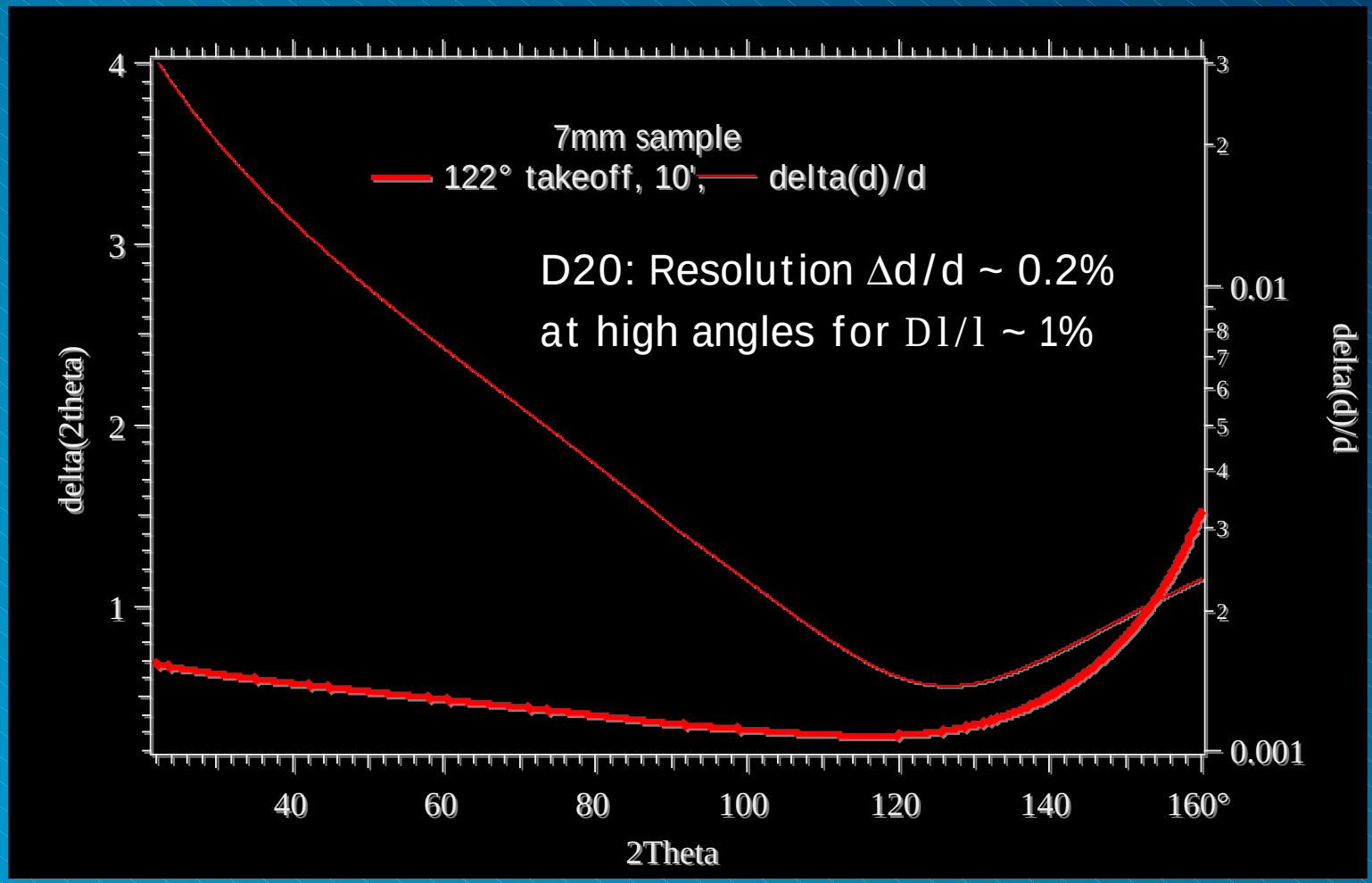
Yes ! Focusing in reciprocal space
can give a factor of x10



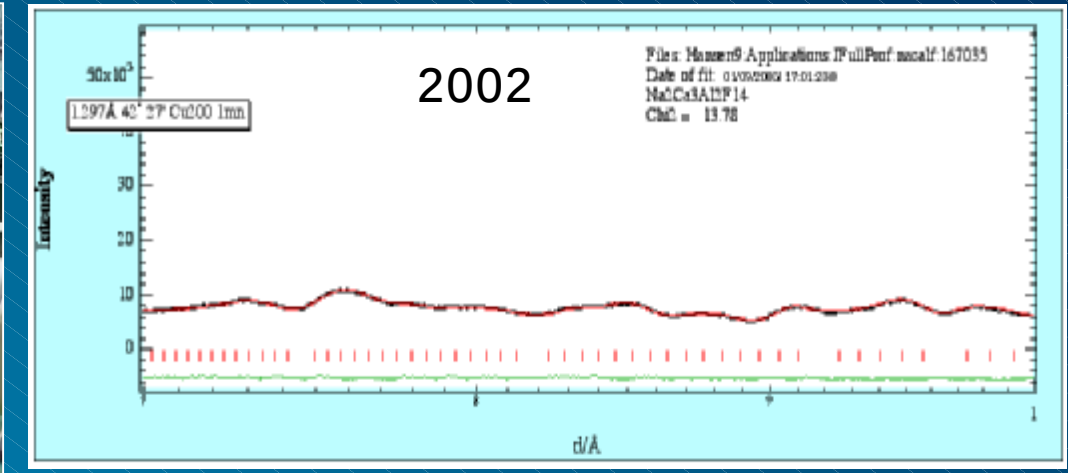
$\Delta d/d \sim 0.1\%$ for $\Delta\lambda/\lambda \sim 1\%$
cf TOF $\Delta d/d \sim \Delta\lambda/\lambda$

Does large Dl/l mean low resolution ?

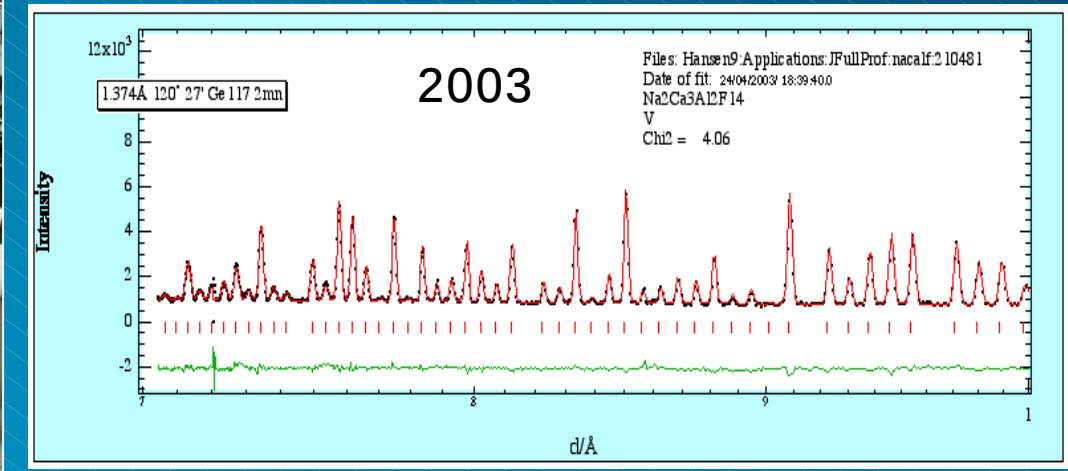
A: No. Resolution is INDEPENDENT of $\Delta\lambda/\lambda$ at focusing angle.



D20 – Good Resolution but still very fast



Before and After (data in 2 min.)

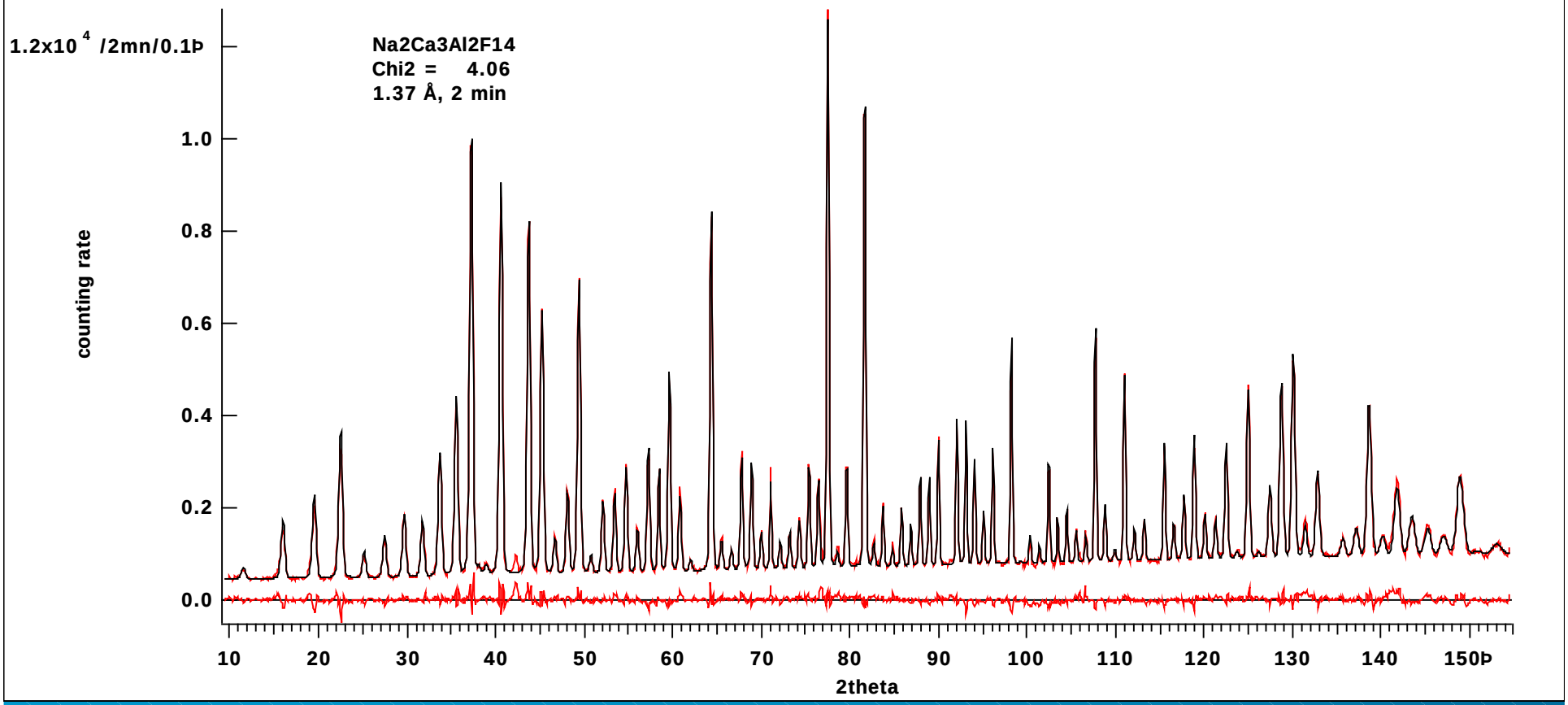


Higher D20 resolution since 2003

D20 – Good Resolution but still very fast

Thomas Hansen (2003) ILL News, June 2003

2 minute D20 data for a ~700 mm^3 sample of $Na_2Ca_3Al_2F_{14}$



GEM at ISIS, comparable to D20

Radaelli, Hammon & Chapon (2003) Neutroni e Luce di Sincrotrone

~700 minute GEM data for a 2mm^3 sample of $Y_3Al_5O_{12}$

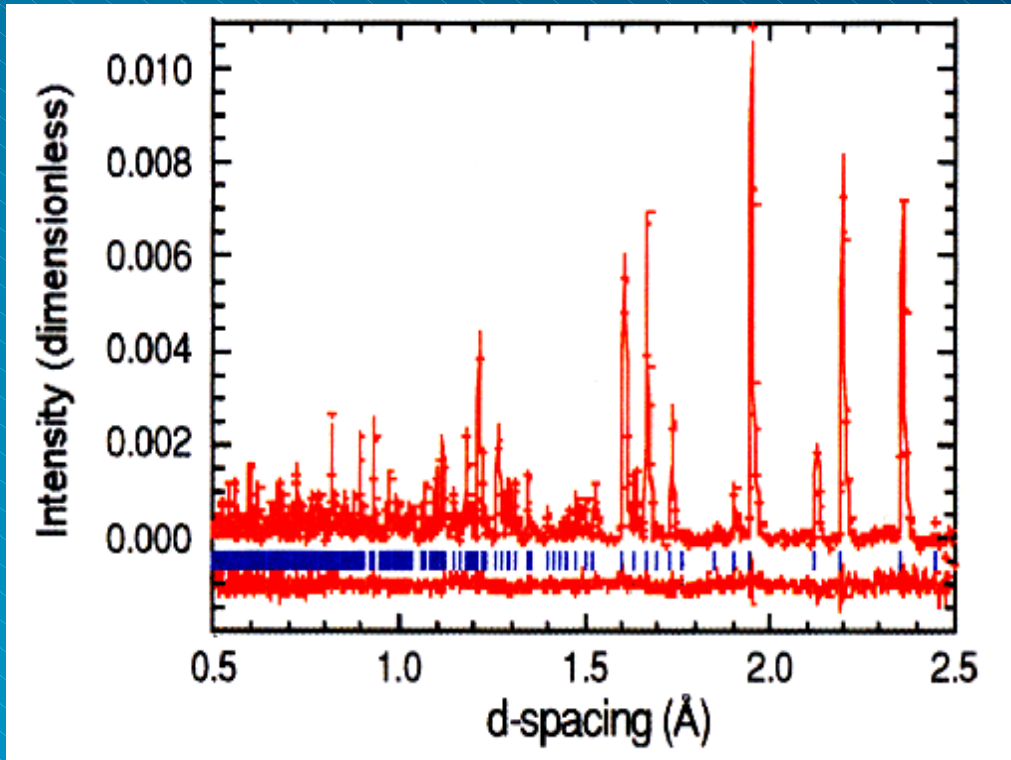
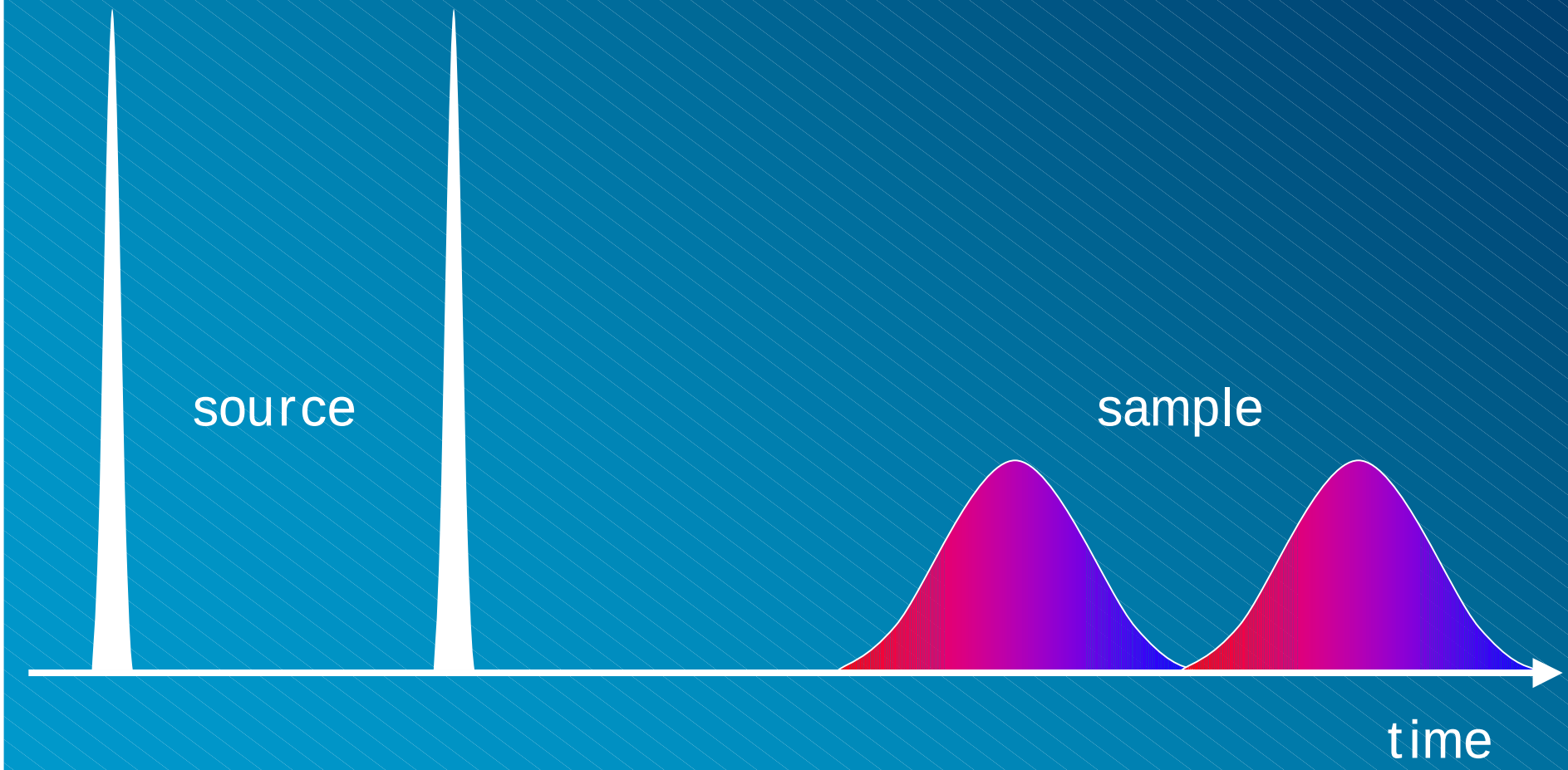


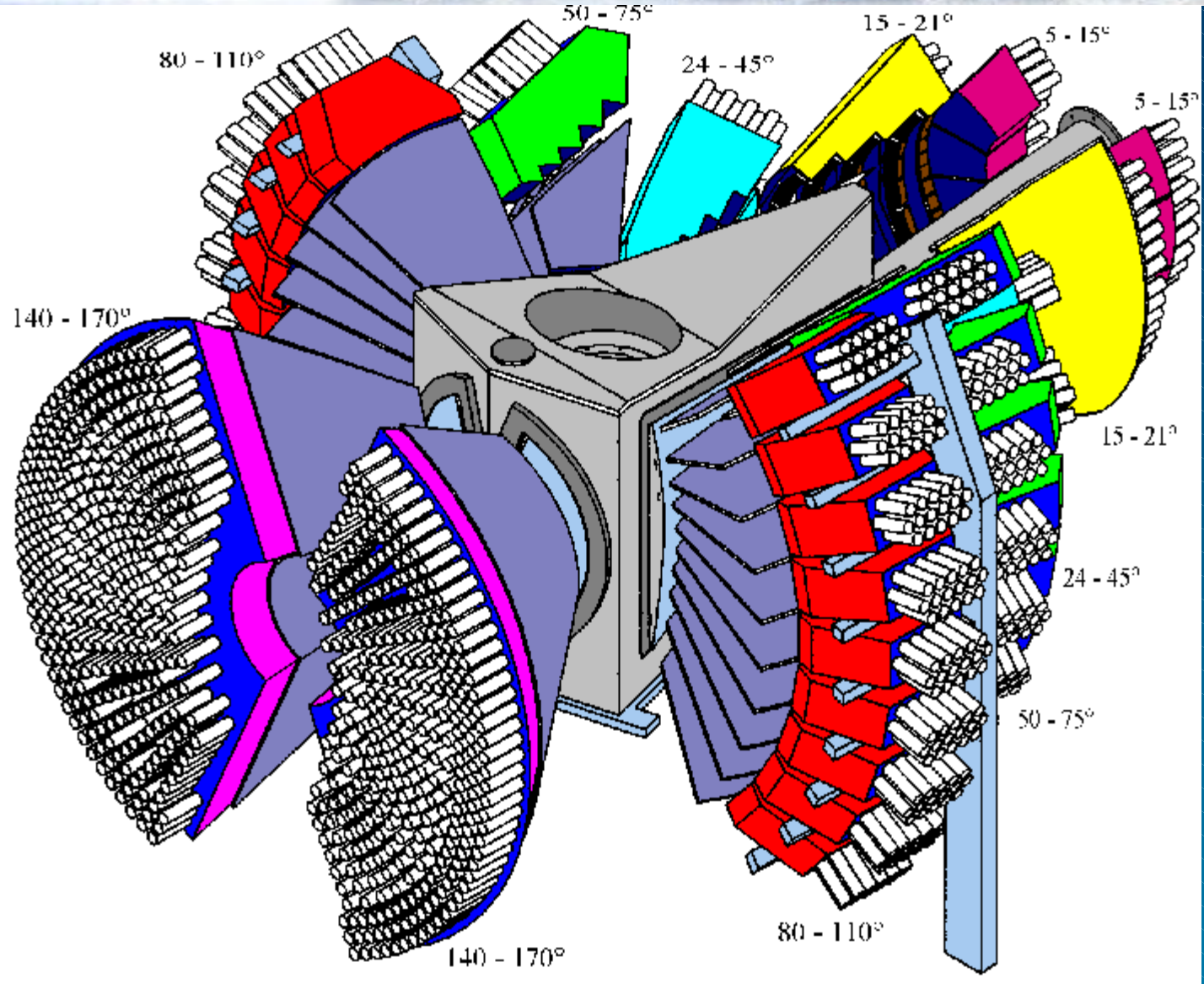
Fig. 7. Rietveld Refinement plot for a 2 mm^2 sample of Yttrium Iron Garnet (YAG), after an overnight data collection.

Why is sample flux low on a pulsed source ?

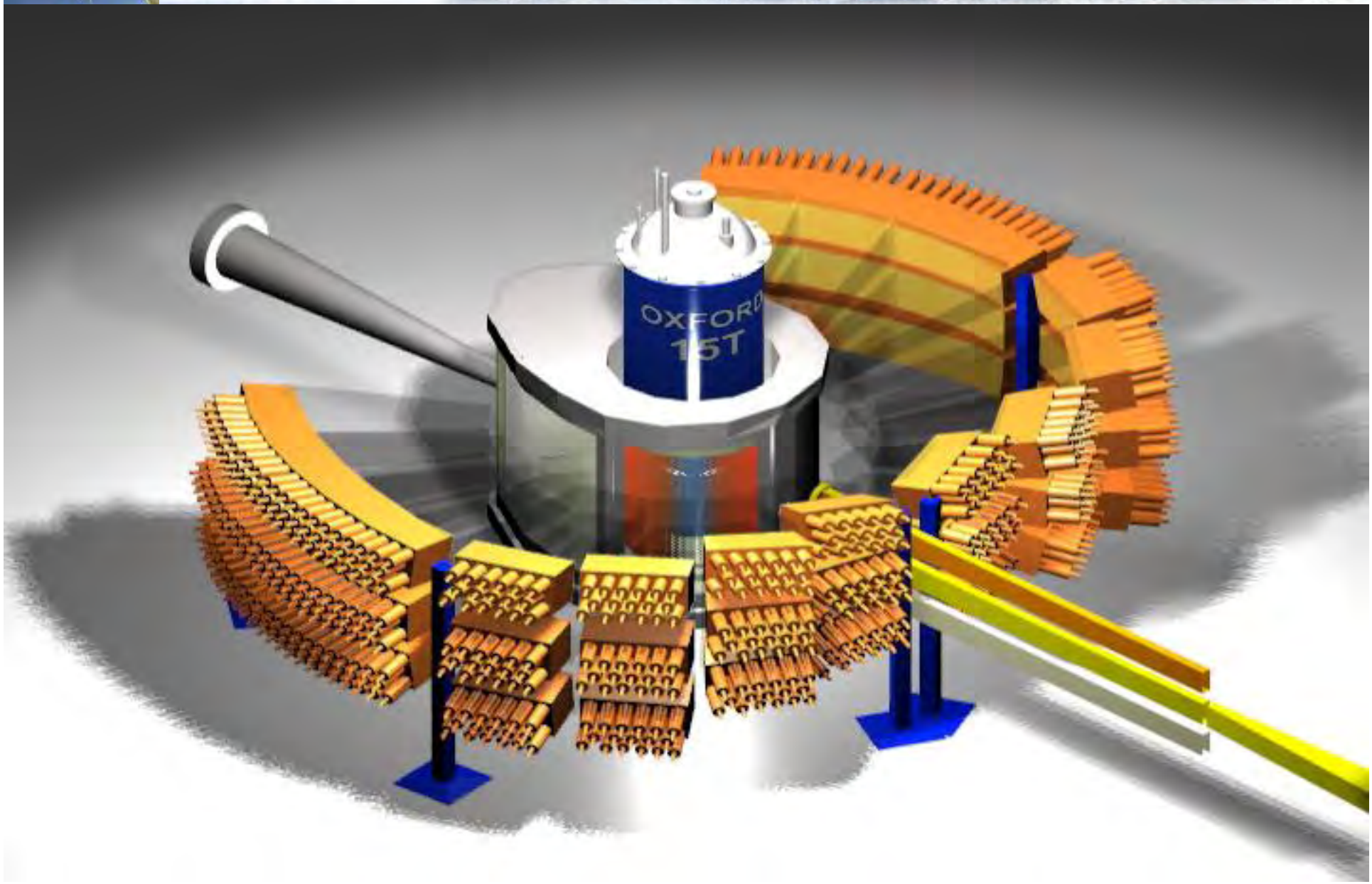
A: The sharp white peaks spread out in wavelength with time
TOF machines have rather constant (low) flux at sample



TOF machines need big detectors
GEM Powder Diffractometer, TS1-ISIS

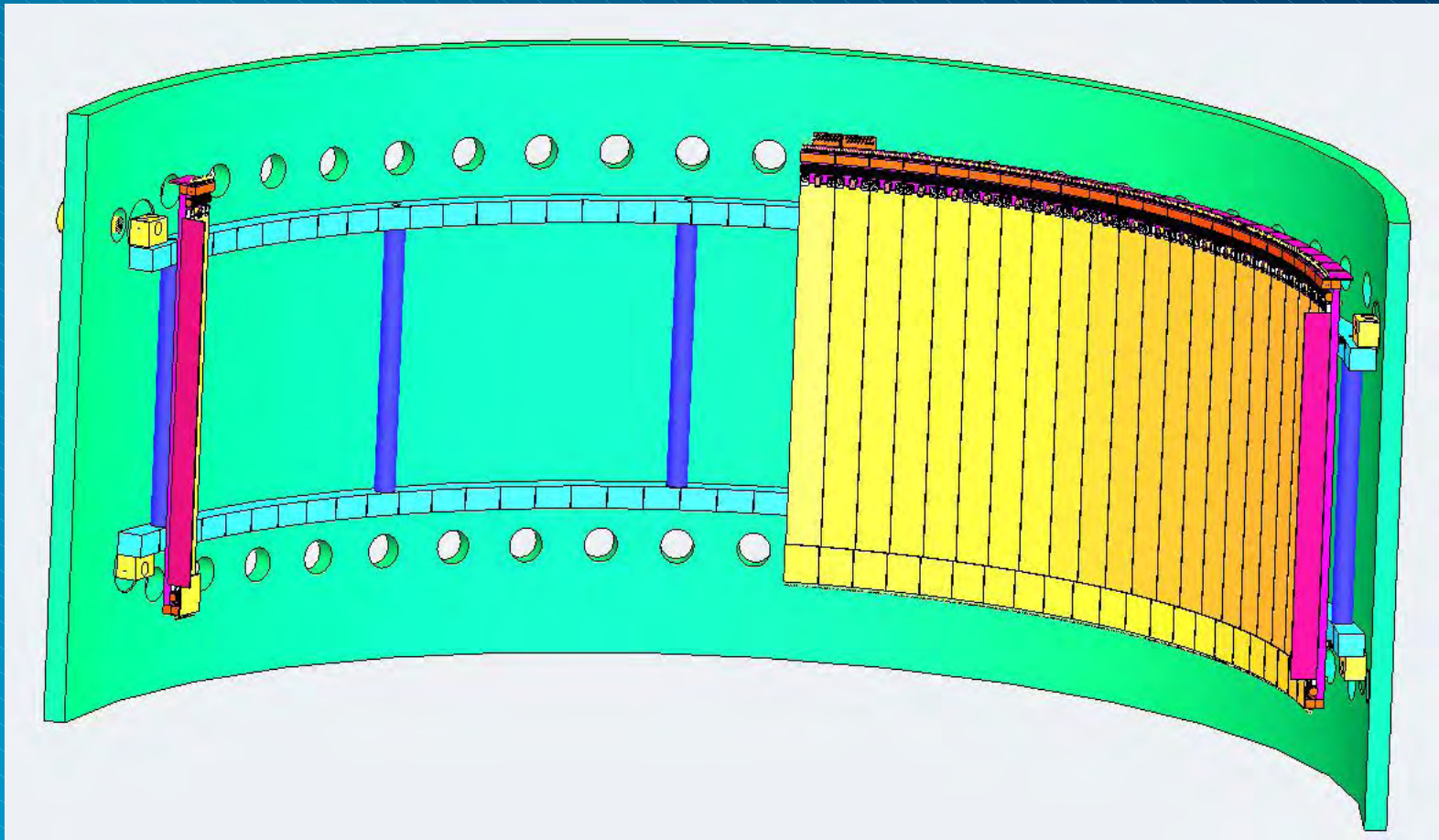


TOF machines need big detectors
GEM Powder Diffractometer, TS1-ISIS



Can we have a big detector too please?

D19 Millennium - A Revolution in large 2D Gas Detectors



2D with Solid Angle > 1 steradian c.f. 0.27 on D20

Comparison of TOF & CW Diffractometers

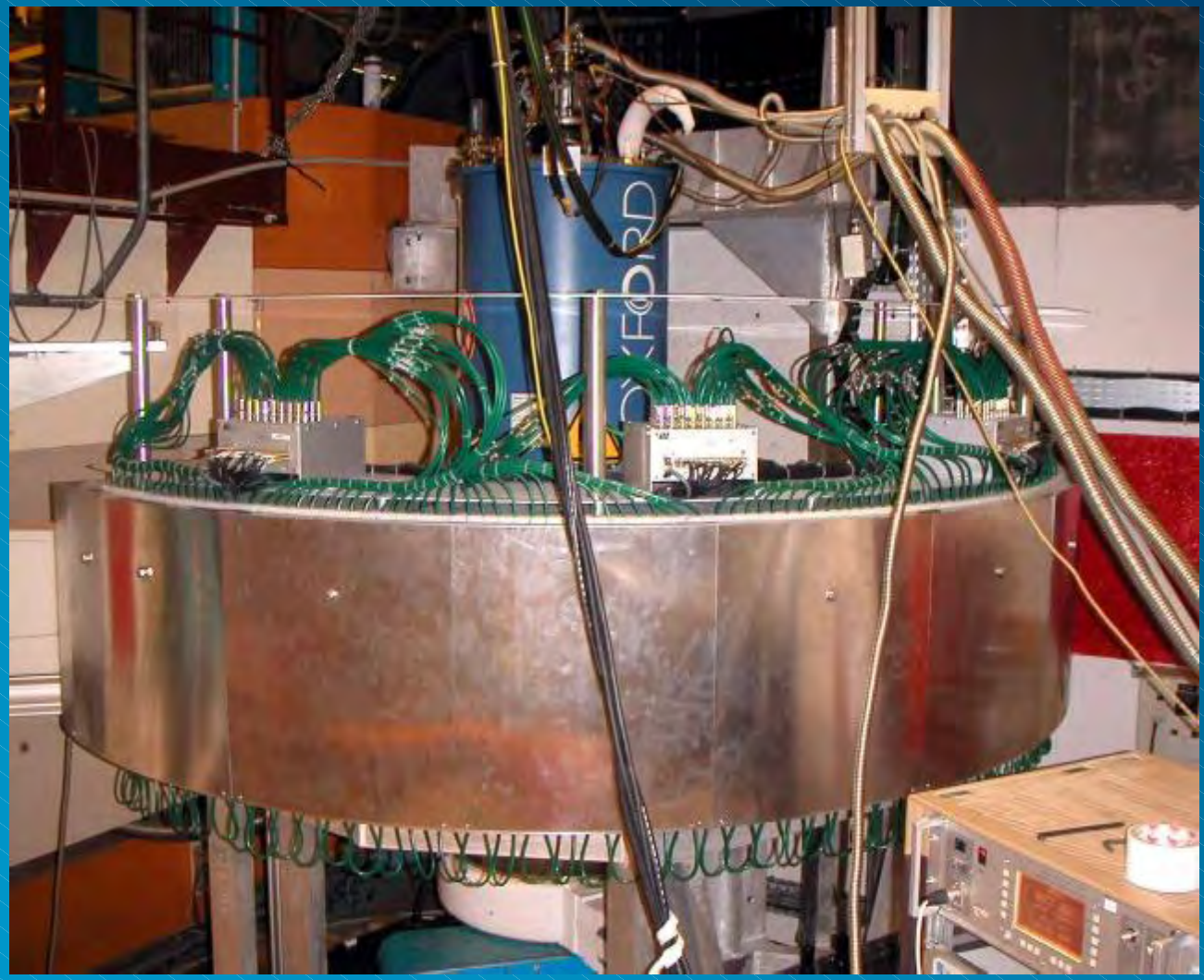
The time-averaged Flux*Detector criterium

	D20	GEM	DRACULA	SNS
time averaged sample flux	$5x10^7$	$\sim 2x10^6$	$\sim 10^8$	$\sim 2.5x10^7$
detector solid angle	0.27 sr	4.0 sr	1.5 sr*	3.0 sr
efficiency	1.7	1	18	9

* Based on new D19 detector: R=760 mm, h=400 mm, 800 linear resistive wires $30^o x 160^o$

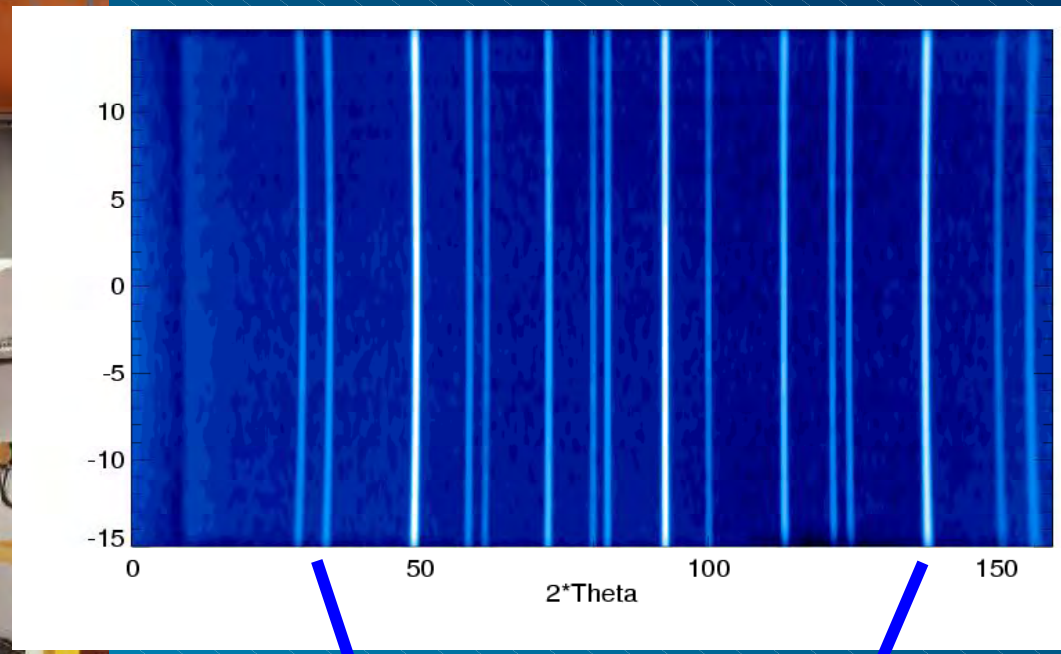
Can we use a big 2D detector for Powders?

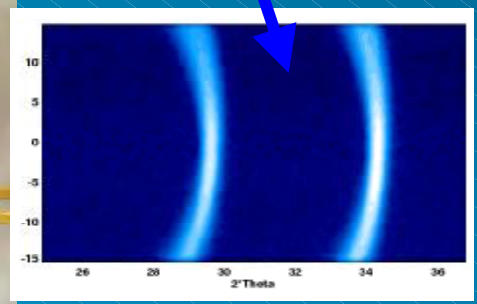
Array of linear wire PSD-tubes on Super-D2B at ILL

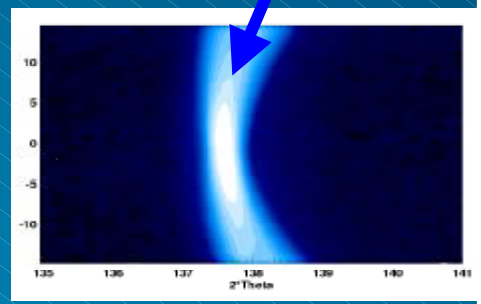


2D detectors for CW Powder Diffraction

UK-EPSRC Super-D2B project at ILL

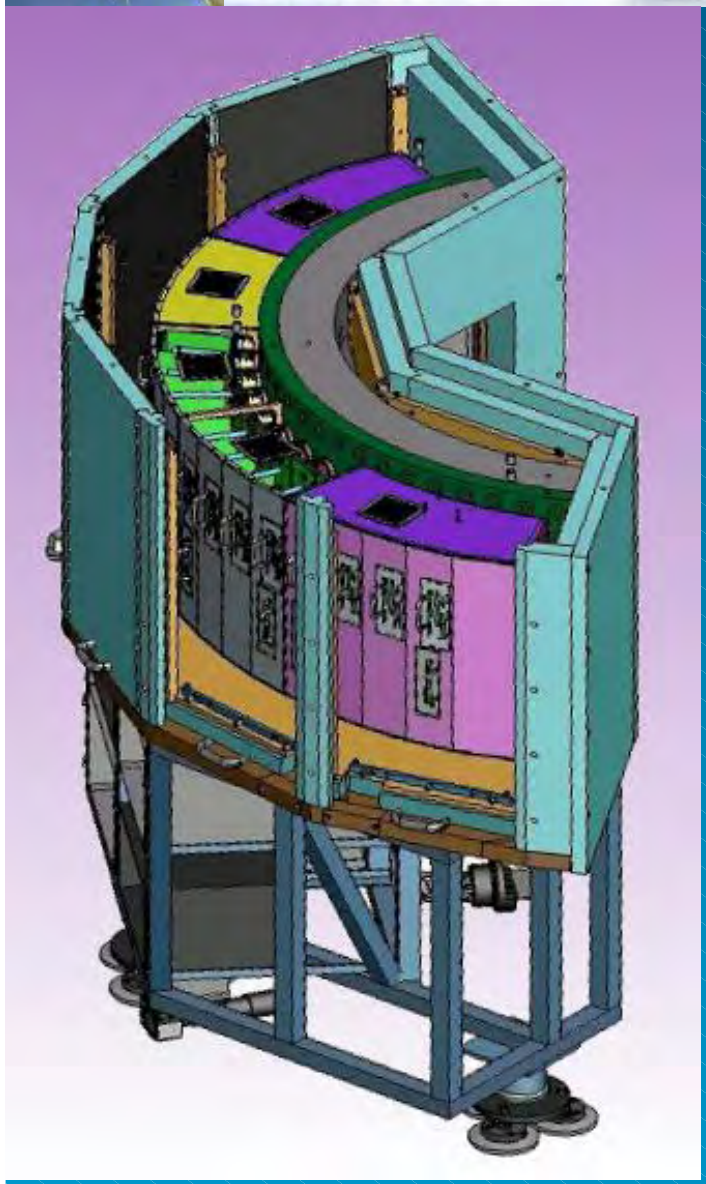




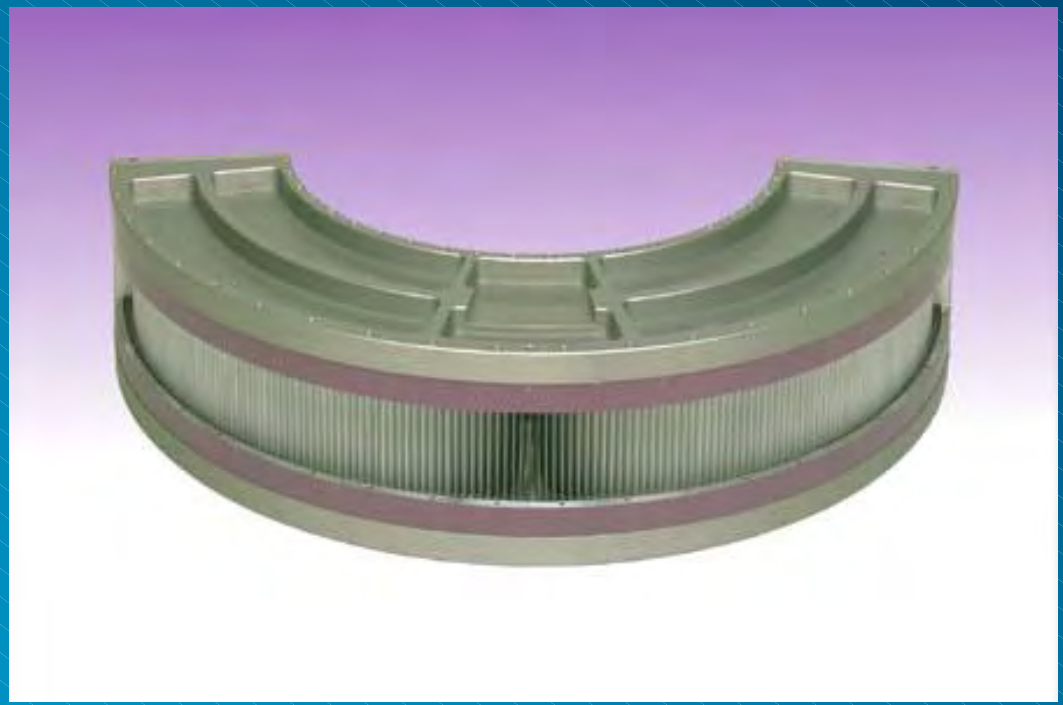


E.Suard, C.Ritter, A.Hewat, P.Attfield… (Edinburgh)

DRACULA - What do we want to do ?



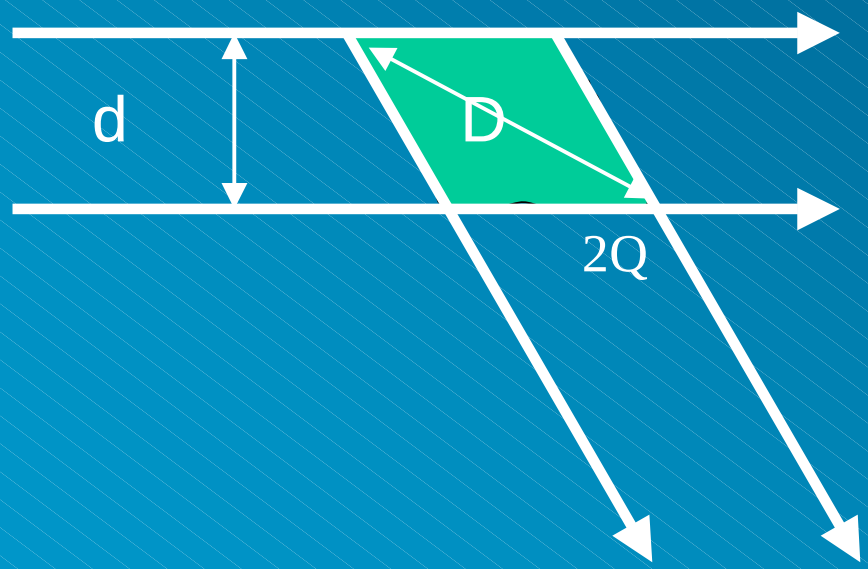
- Order of magnitude smaller samples than D20
- Low background (pressure cell)
- Large, compact 2D area detector (cf D19)
- Radial collimator



DRACULA – Small Samples, Low Background

Large detector & radial collimator near 90º scattering

± 15º vertical as for the new D19 detector cf ±7º for new Paris-Edinburgh cell
± 30º horizontal ie 2Q = 60º - 120º (range of scattering angles for pressure cell)



d = diameter of the incident beam
D = diameter of scattering volume
= d/sinQ
= dÖ2 (minimum at 2Q = 90º)
= 2d (maximum at 2Q = 60º & 120º)

D = 5mm – 7mm for 2Q = 60º - 120º

Scattering limited to a very small sample volume

DRACULA – Small Samples, Low Background

Can we obtain all d-spacings with a 2Q range of 60º-120º ?
(i.e. with a very small scattering volume)

Use a large focusing Ge monochromator near 90º to obtain several l

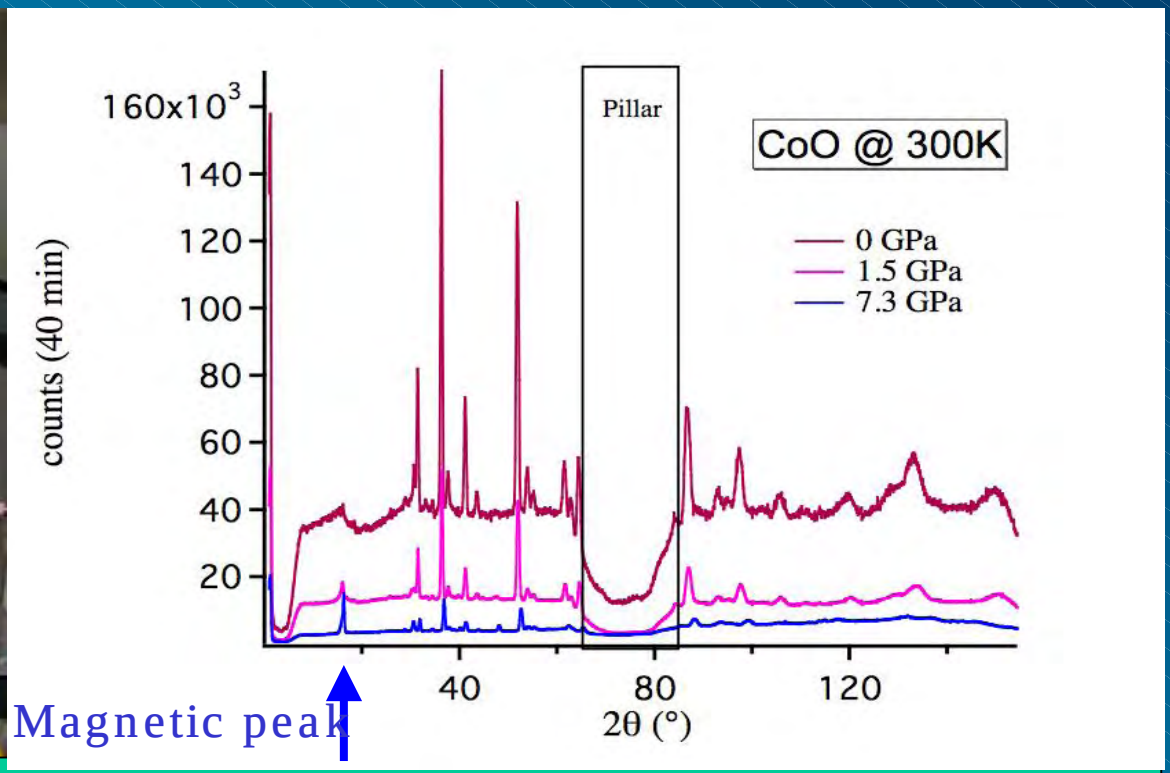
[115] -> 1.54Å;		d= 0.889Å - 1.54Å
[113] -> 2.44Å;	(graphite filter)	d= 1.39Å - 2.44Å
[111] -> 4.61Å;	(beryllium filter)	d= 2.66Å - 4.61Å

Applications - fast detectors, small samples

D20 with "large" Paris-Edinburgh Pressure Cell (50 Kg)

Kernavanois et al. (2003) Advanced Millennium Pressure Project

40 minute D20 data for a 100 mm^3 sample of CO at 7.3 GPa



BUT low temperatures –> smaller cells -> 1-10 mm^3 samples

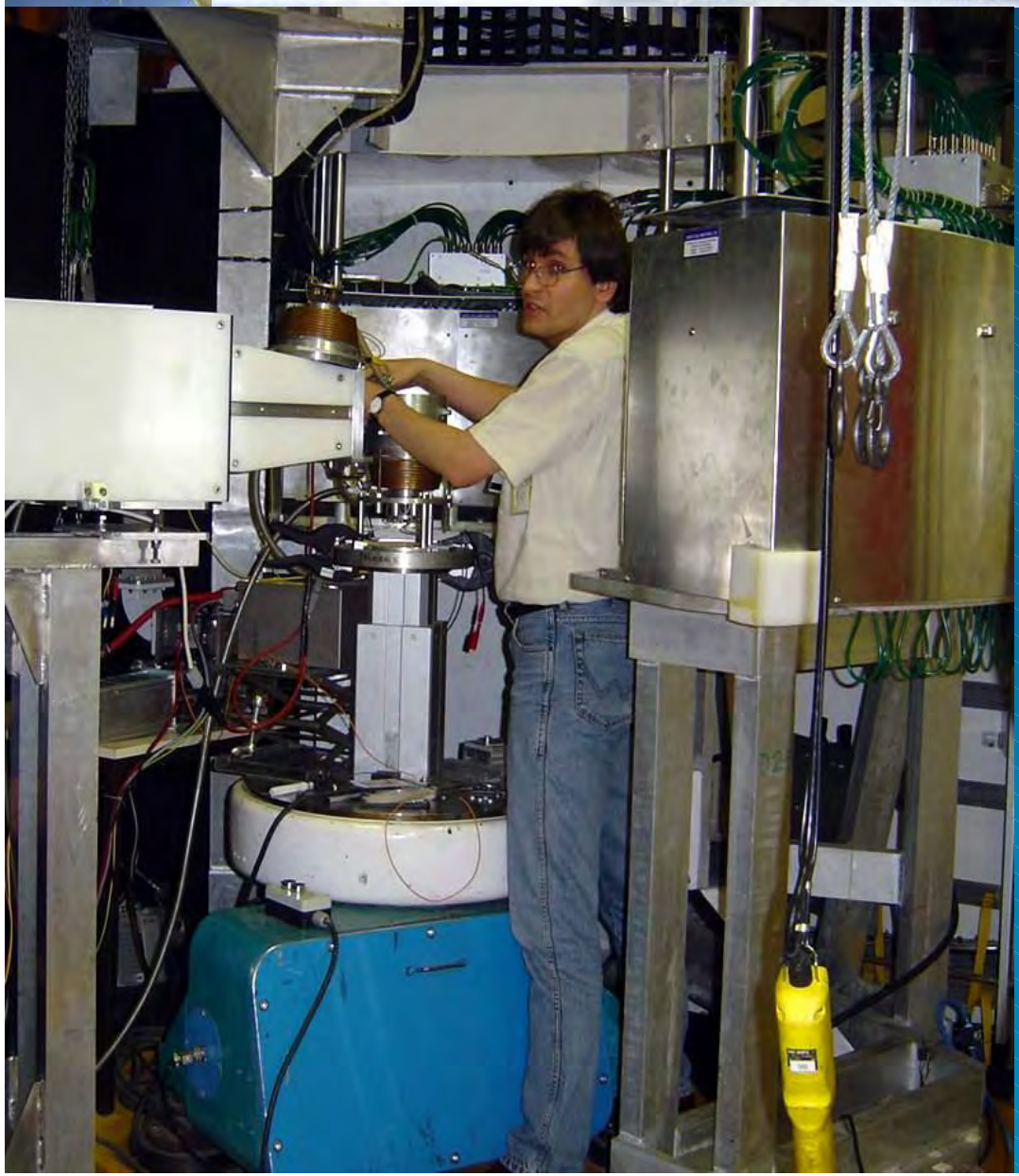
Applications - fast detectors, small samples

Very fast chemical and electrochemical kinetics

- The explosive SHS reaction was studied in real time with neutrons
- The reaction is exothermic, & heats the sample to 2200°C in <1 sec
- The complete diffraction pattern (left) is collected at 300 ms intervals - A World Record

D.Riley, E.Kisi, T.Hansen, A.Hewat (2002)

Applications - fast detectors, small samples



High-T Microwave Furnace Super-D2B (Boysen et al.)

…with Carsten Korte from Giessen (2004)

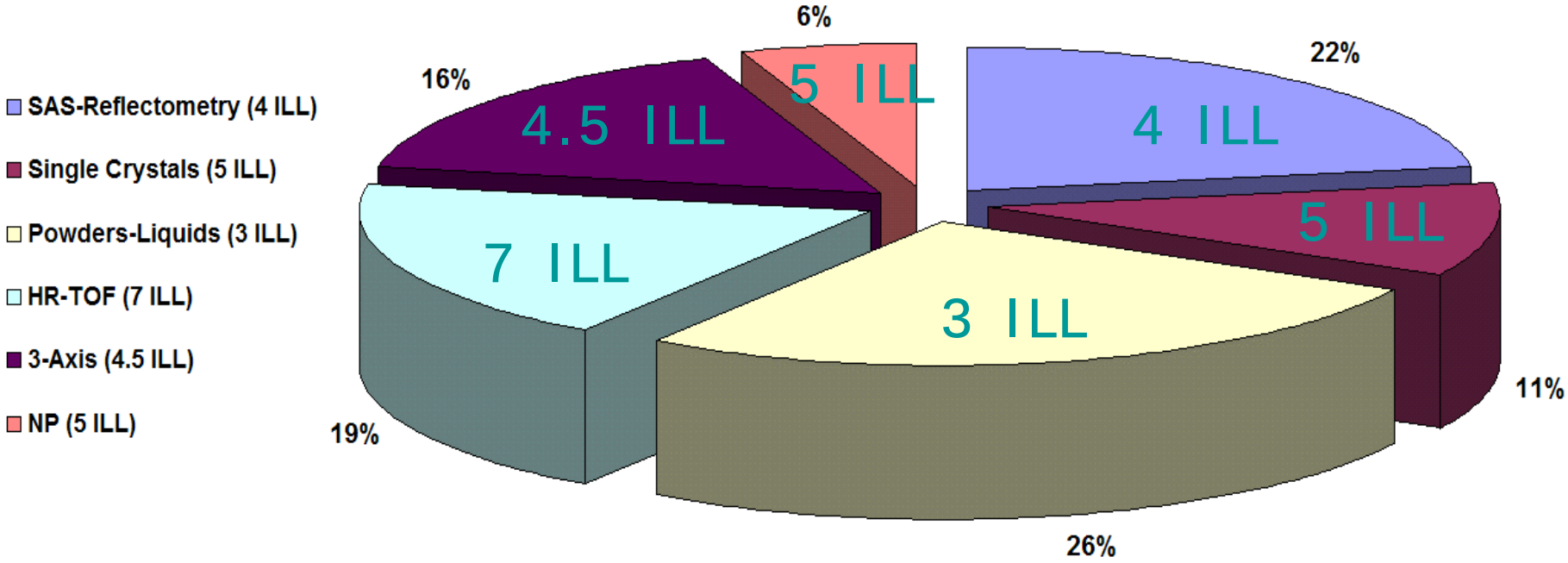
DRACULA–Why do we need a new machine ?

Convert D20 to DRACULA ?

- D20 has only recently been finished & is now working well
- D20 is the ILL's most requested machine (57 proposals)
- Only 2 modern powder machines for 22% of all proposals

DRACULA–Why do we need a new machine ?

Only 3 ILL machines for more than ¼ of all ILL proposals



D2B, D4, D20

ESS ambitions for powder diffraction

Proposed ESS Powder Diffractometers

- ST05 High-Q Powder Diffractometer HQP
- ST06 Liquids & Amorphous Diffractometer LAD
- SM10 Single Pulse Diffractometer SPD
- SD17 Magnetic Powder Diffractometer MagP
- SD18 High Resolution Powder Diffractometer HRPD
- LM05 Ultra-high Resolution Powder Diffractometer URPD
- LM06 High Pressure Powder Diffractometer HiPD

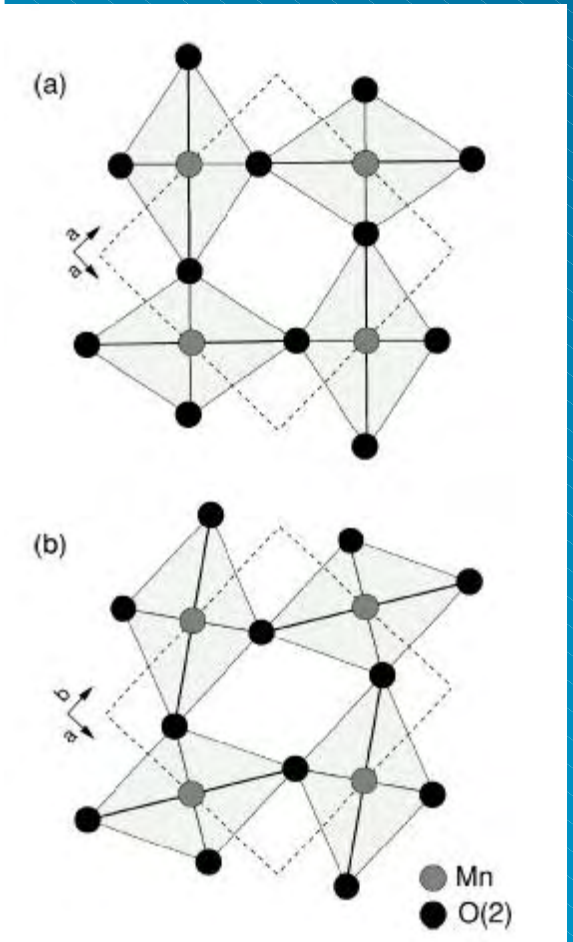
What might we do while waiting for ESS ?

ILL 2-axis diffractometers that might use large 2D detectors

- **High intensity, small sample powder diffractometer DRACULA**
- **Liquids & Amorphous Materials Diffractometer super-D4**
- **Long Wavelength Magnetism/Biology Diffractometer super-D16**

Measurement of the local Jahn-Teller distortion in $LaMnO_{3.006}$

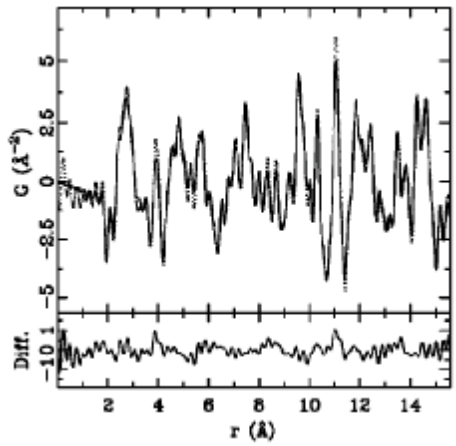
Th. Proffen, R. G. DiFrancesco, and S. J. L. Billinge (1999) **60**, 9973

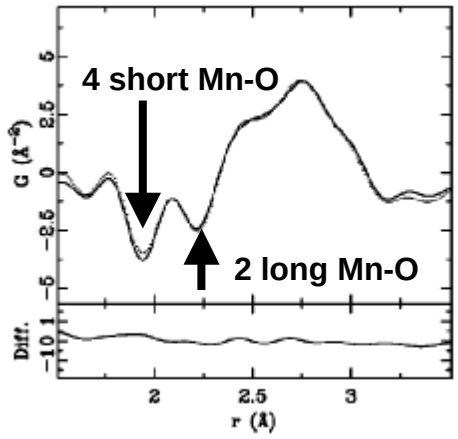


- Rietveld -> Average structure
- PDF -> Local details

- Rietveld NPD -> CMR distortion
- PDF -> Confirms JT distortion

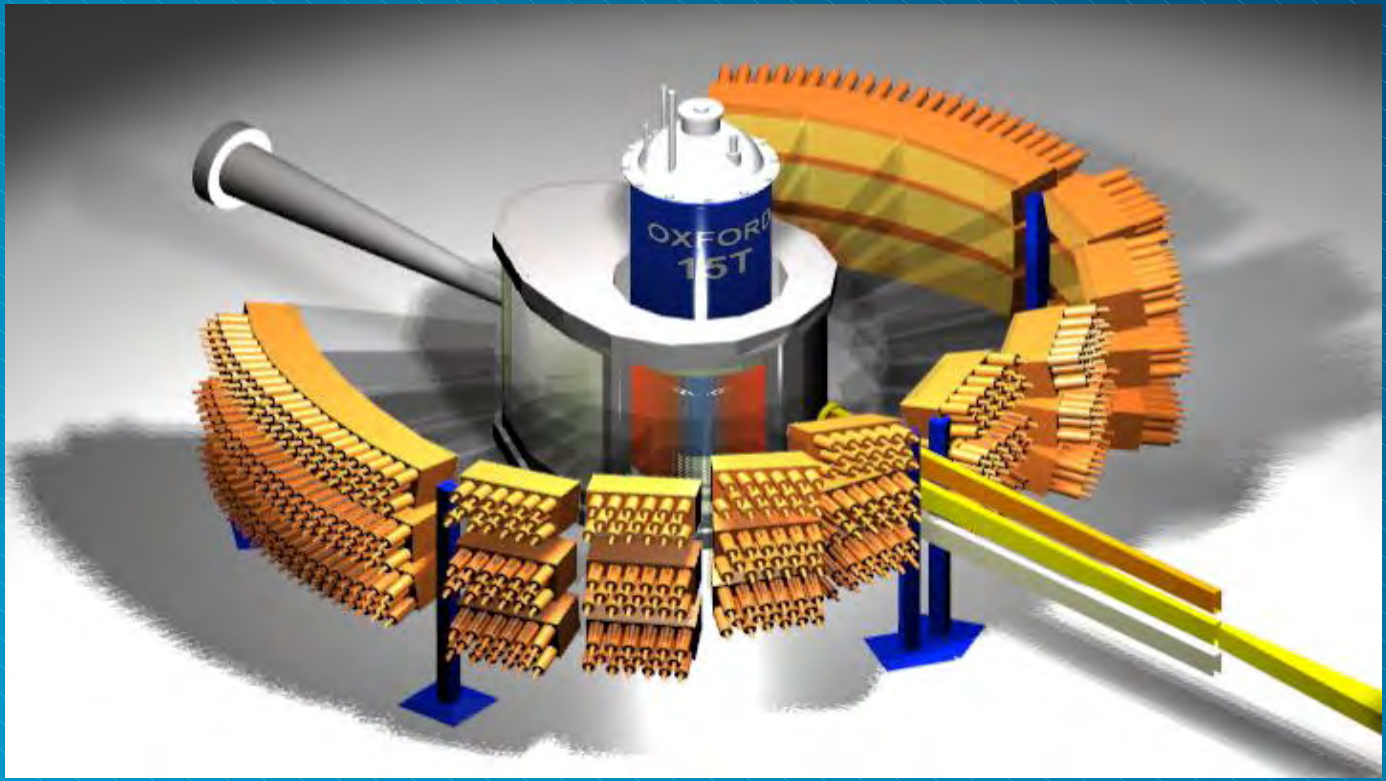
- PDF is increasingly important
- Super-D4/D9 diffractometer





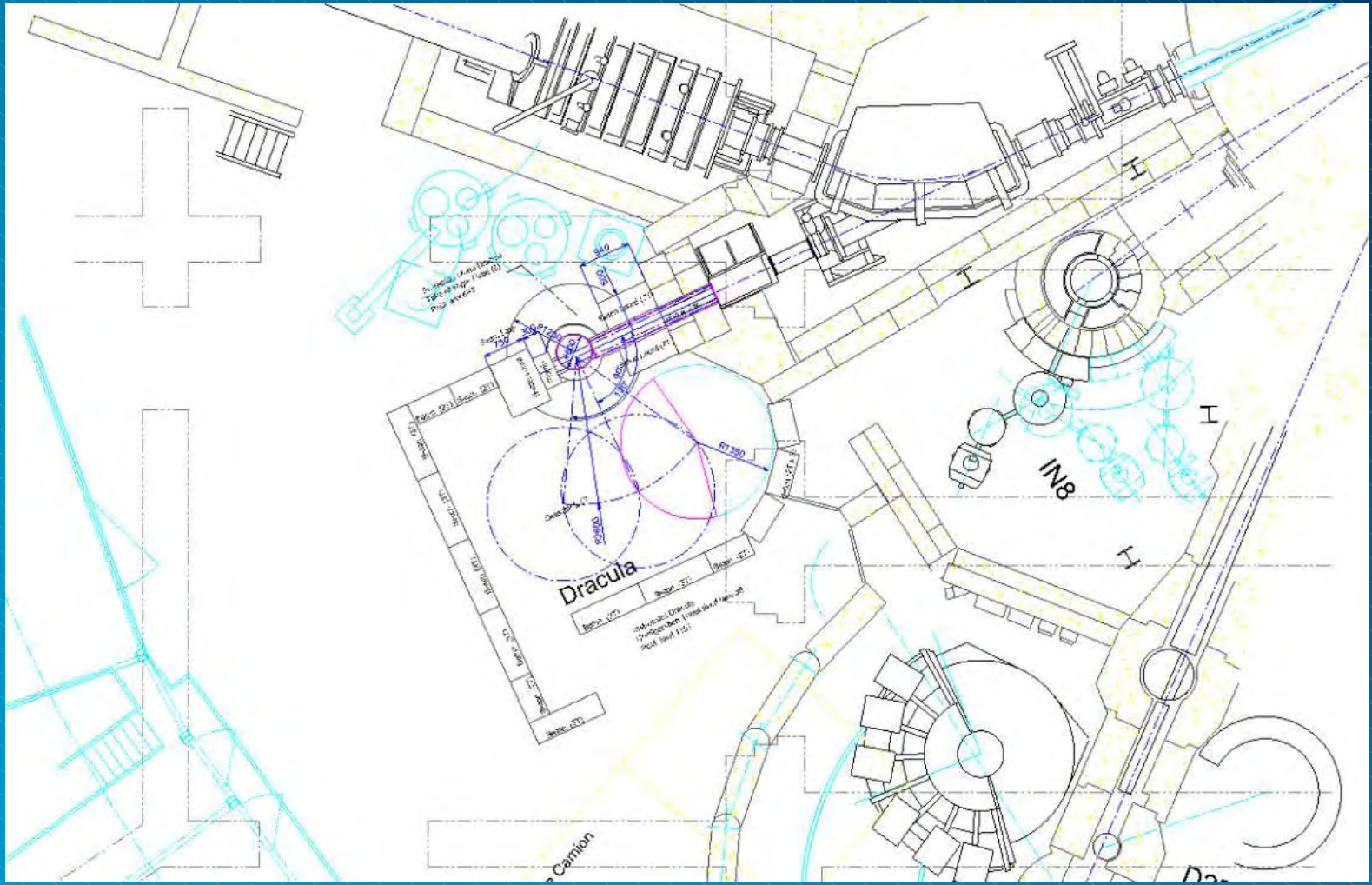
Magnetism and Biology Dracula (super-D16)
High resolution with long wavelengths

- ILL lacks a wide-angle, cold neutron machine like ISIS-WISH
- WISH is designed for long-period structures – magnetism & biology
- D16 is a good candidate – exists already, 90º take-off, long l.
- Replace current small "bidim" on D16 by large D19-type banana ?



Thermal DRACULA on a High Flux Beam

DRACULA on H9 (replacing the Tomography station)



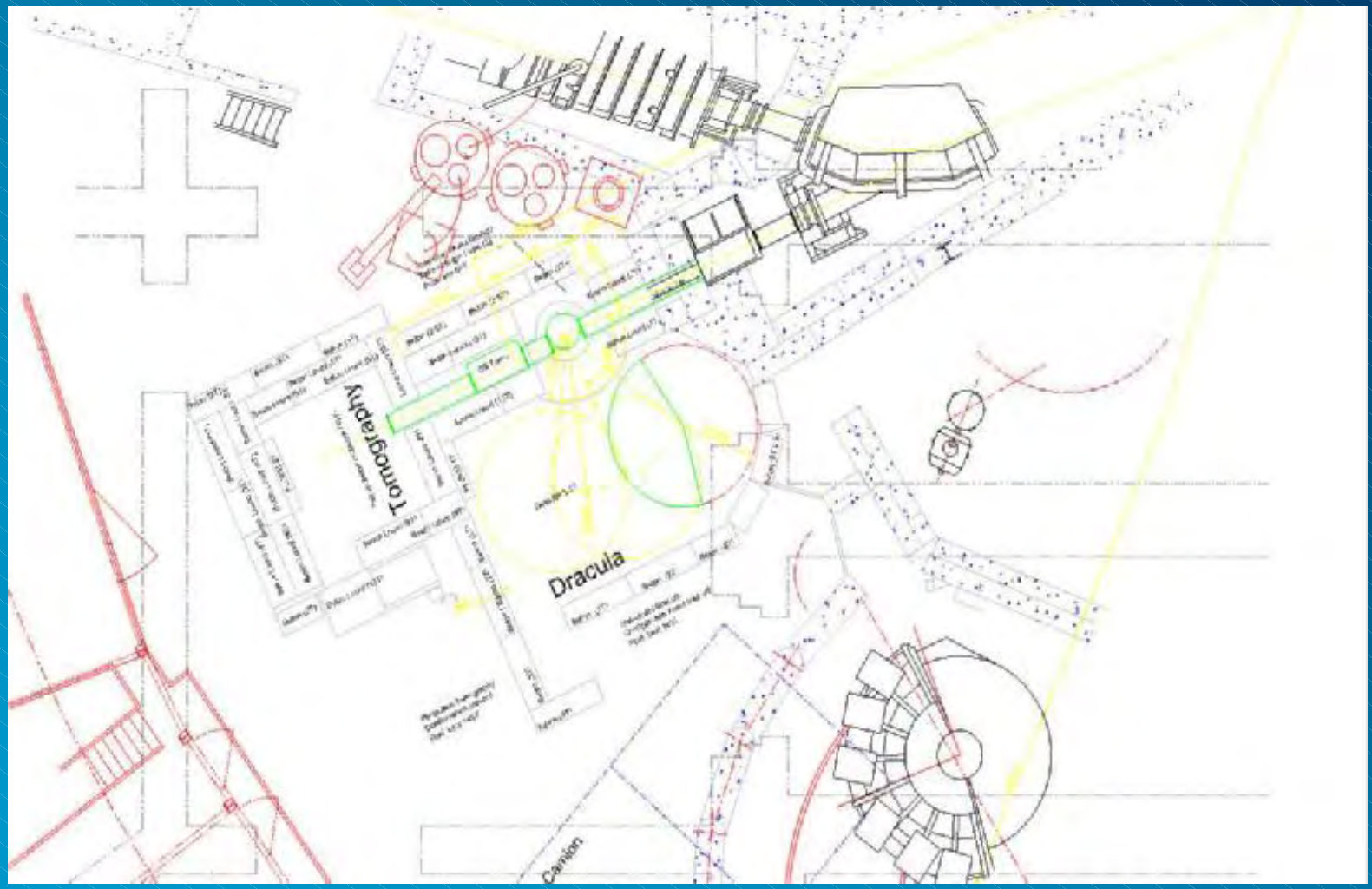
Thermal DRACULA on a High Flux Beam

DRACULA on H9 (replacing the Tomography station)

- Dracula would weigh about the same as Tomography
- Dracula slightly restricted by Lohengrin chariot/magnet
- But the big intensity gain comes from wavelength focussing
- For that, we need a wide monochromator, not so tall
- But it would be nice to find a place for tomography…

Thermal DRACULA on a High Flux Beam

DRACULA on H9 (co-existing with Tomography station?)



Thermal DRACULA on a High Flux Beam

DRACULA on H9 (co-existing with Tomography station?)

- Tomography would be moved back ~4m
- Tomography could be supported using a pillar in level-B
- A detailed floor load calculation has been commissioned
- Tomography would benefit by having better resolution
- Tomography would benefit from a better, larger casemate
- Dracula monochromator would absorb ~15% of white beam

DRACULA cost and feasibility

- Dracula would use tested D19-type 2D-detector
- Dracula would also be useful for non-powder diffraction
- Dracula casemate optics would be similar to that of D20
- Dracula mono. would be less high, but horizontally focussing
- Cost and time-scale for Dracula can be easily calculated
- Dracula is a “no-risk” project that will give ILL a big lead

DRACULA – Strategy or Submission ?

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Can we compete with the Americans while waiting for ESS?

(Free Advice to ILL Directors)

- Use our natural advantage – time average flux on sample
- Use big detectors, as on pulsed neutron sources
- Do not assume that the SNS will be a long time coming
- Do not wait until the SNS is operational before reacting