DRAC or DRACULA?

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*Diffractionometer 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

1B - Disordered Mat'ls Diffractometer – DOE Funded (SING) – Commission 2010

18 - Wide Angle Chopper Spectrometer – IDT DOE Funded – Commission 2007

17 - High Resolution Chopper Spectrometer – DOE Funded (SING) – Commission 2008

3 - High Pressure Diffractometer – DOE Funded (SING) – Commission 2007

15 - Spin Echo

2 - Backscattering Spectrometer – SNS Funded – Commission 2006


5 - Cold Neutron Chopper Spectrometer – IDT DOE Funded – Commission 2007

6 - SANS – SNS Funded – Commission 2007

9 - Engineering Diffractometer – IDT CFI Funded – Commission 2008


12 - Single Crystal Diffractometer – DOE Funded (SING) – Commission TBD

13 - Fundamental Physics Beamline – IDT DOE Funded – Commission TBD

14B - Hybrid Spectrometer – DOE Funded (SING) – Commission 2011

? - Chemical Spectrometer

60 m
SNS-EFAC recommendations

1. “...the SNS should immediately begin work on the conceptual design for... a third generation powder diffractometer with a resolution $\Delta d/d$ of $\sim1\times10^{-3}$ at 90°.” Nov 1998. 
Note: Moderately high resolution at 90° scattering.

1. “SNS without a world-class powder diffractometer on day one is unthinkable.” May 2001.

1. “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
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?
Proposed ESS Powder Diffractometers

<table>
<thead>
<tr>
<th>ST05</th>
<th>High-Q Powder Diffractometer</th>
<th>HQP</th>
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</thead>
<tbody>
<tr>
<td>ST06</td>
<td>Liquids &amp; Amorphous Diffractometer</td>
<td>LAD</td>
</tr>
<tr>
<td>SM10</td>
<td>Single Pulse Diffractometer</td>
<td>SPD</td>
</tr>
<tr>
<td>SD17</td>
<td>Magnetic Powder Diffractometer</td>
<td>MagP</td>
</tr>
<tr>
<td>SD18</td>
<td>High Resolution Powder Diffractometer</td>
<td>HRPD</td>
</tr>
<tr>
<td>LM05</td>
<td>Ultra-high Resolution Powder Diffractometer</td>
<td>URPD</td>
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<tr>
<td>LM06</td>
<td>High Pressure Powder Diffractometer</td>
<td>HiPD</td>
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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.
The average count rate is the product of:

- the flux at the sample
- the detector solid angle and efficiency
- the sample volume
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.
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).
Efficiency for a given resolution \( = \) \( \frac{\text{time averaged flux on sample} \times \text{sample volume} \times \text{detector solid angle}}{} \)


“Scientific opportunities with advanced facilities for neutron scattering”
Shelter Island Workshop, 1984
### Comparison of TOF & CW Diffractometers

#### The time-averaged Flux*Detector criterium

D20 has high flux, GEM has a big detector

<table>
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The time-averaged Flux*Detector criterium

So, let’s use a big detector too!

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* Based on new D19 detector: $R=760$ mm, $h=400$ mm, 800 linear resistive wires $30^\circ \times 160^\circ$
The time-averaged Flux*Detector criterium

Only then can we compete with the SNS.

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* Based on new D19 detector: R=760 mm, h=400 mm, 800 linear resistive wires $30^\circ \times 160^\circ$
Why is sample flux so high from a reactor?

A: Large vertically focusing monochromators?

No! Focusing in real space only gives a factor of \( x^2 \) or \( x^3 \)

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

Monochromator Source

Detector Sample

$\frac{\Delta d}{d} \sim 0.1\% \text{ for } \frac{\Delta \lambda}{\lambda} \sim 1\%$

cf TOF $\frac{\Delta d}{d} \sim \frac{\Delta \lambda}{\lambda}$

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
Does large $\Delta \lambda/\lambda$ mean low resolution?

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

D20: Resolution $\Delta d/d \sim 0.2\%$

at high angles for $\Delta \lambda/\lambda \sim 1\%$
D20 – Good Resolution but still very fast

Before and After (data in 2 min.)

Higher D20 resolution since 2003

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004

2 minute D20 data for a ~700 mm³ sample of Na₂Ca₃Al₂F₁₄

D20 - Good Resolution but still very fast

Chi² = 4.06
1.37 Å, 2 min

Na₂Ca₃Al₂F₁₄

1.2×10⁴ /2mn/0.1°

1.0

0.8

0.6

0.4

0.2

0.0

10 20 30 40 50 60 70 80 90 100 110 120 130 140 150°

2θ

counting rate

~700 minute GEM data for a 2mm³ sample of Y₃Al₅O₁₂

Fig. 7. Rietveld Refinement plot for a 2 mm² 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

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* Based on new D19 detector: R=760 mm, h=400 mm, 800 linear resistive wires 30°x160°
Can we use a big 2D detector for Powders?

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

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
2D detectors for CW Powder Diffraction

UK-EPSRC Super-D2B project at ILL

E. Suard, C. Ritter, A. Hewat, P. Attfield... (Edinburgh)
Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
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
Large detector & radial collimator near 90° scattering

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

\[ d = \text{diameter of the incident beam} \]
\[ D = \text{diameter of scattering volume} \]
\[ = \frac{d}{\sin(\theta)} \]
\[ = d\sqrt{2} \text{ (minimum at } 2\theta = 90°) \]
\[ = 2d \text{ (maximum at } 2\theta = 60° \text{ & } 120°) \]

D = 5mm – 7mm for 2Θ = 60° - 120°

Scattering limited to a very small sample volume
Can we obtain all d-spacings with a 2θ range of 60°-120°?  
(i.e. with a very small scattering volume)

Use a large focusing Ge monochromator near 90° to obtain several λ

<table>
<thead>
<tr>
<th>Plane</th>
<th>d-spacing</th>
<th>Filter type</th>
<th>d-range</th>
</tr>
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<tbody>
<tr>
<td>[115]</td>
<td>1.54 Å</td>
<td></td>
<td>0.89 Å - 1.54 Å</td>
</tr>
<tr>
<td>[113]</td>
<td>2.44 Å</td>
<td>graphite filter</td>
<td>1.39 Å - 2.44 Å</td>
</tr>
<tr>
<td>[111]</td>
<td>4.61 Å</td>
<td>beryllium filter</td>
<td>2.66 Å - 4.61 Å</td>
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Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
Applications - fast detectors, small samples

D2O with "large" Paris-Edinburgh Pressure Cell (50 Kg)
Kernavanois et al. (2003) Advanced Millennium Pressure Project
40 minute D2O data for a 100 mm$^3$ sample of CO at 7.3 GPa

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

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
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.


Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
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

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
DRACULA—Why do we need a new machine?

Only 3 ILL machines for more than 1/4 of all ILL proposals

- 4.5 ILL: 16%
- 5 ILL: 6%
- 7 ILL: 19%
- 3 ILL: 26%
- 4 ILL: 22%
- 5 ILL: 11%

D2B, D4, D20

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
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$_{3.006}$


- Rietveld -> Average structure
- PDF -> Local details
- Rietveld NPD -> CMR distortion
- PDF -> Confirms JT distortion
- PDF is increasingly important
- Super-D4/D9 diffractometer
- 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, 90° take-off, long λ.
- Replace current small “bidim” on D16 by large D19-type banana?
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?)

Alan Hewat, ILL Presentation of DRACULA, 23 August 2004
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
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