The ILL Diffraction Group

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The ILL Diffraction Group
Alan Hewat, Diffraction Group Leader

1 Magnetism on Mars
1 Levitation at 3000°C
1 Polymer Structures
1 Polarised Eddies
1 Zener Polarons
1 Reciprocal Space Explorer

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Questions from the Science Council (E. Forgan)

- Is the present arrangement of Instrument Groups best?
- Is your group coherent or not and does it matter?
- Overlap between Colleges and Instrument Groups?
- Compare/contrast with present and future pulsed sources?
- Are your instruments up to competing reactor sources?
- Is there a place for "workhorse" instruments at the ILL?
- Do you have proposals that involve new beam positions?
- Would instruments benefit from an end-beam position?
- What things could you give up to allow new developments?
- What other factors are seriously limiting performance? (e.g. sample environment, long timescales for delivery...)

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Where are we now?

Where are we going?
SNS
And the Competition?

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ILL Diffraction instruments can be divided into 3 groups:

1. **Thermal Single Crystal Diffractometers:**
   - **D10**: Magnetism/structure, energy resolution & spec. environ.
   - **D19**: Large molecules, fibres, polymers, in chemistry & biology.
   - **VIVALDI**: Reciprocal space surveys, phase T/Ns, v. small crystals.

2. **Thermal Powder Diffractometers:**
   - **D1A (50%)**: Rietveld refinement, medium size structures, strain.
   - **D2B**: High resolution, high flux, subtle structural changes.
   - **D20**: High flux, chemical kinetics, simple magnetic structures.

3. **Hot Source Diffractometers:**
   - **D3**: Complex magnetic structures, spin, polarised neutrons.
   - **D4 (50%)**: Liquids & amorphous structures.
   - **D9**: High-resolution of atomic structures, complements D3.
Other ILL Diffraction projects/responsibilities:

1. SALSA strain scanner - new EPSRC financed project  
   Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)

2. FaME38 Engineering Lab. - new EPSRC financed project  
   P. Webster et al. (Salford)

3. Crystal Alignment Machine - new test machine for all ILL  
   B. Ouladdiaf

4. $^3$He cell for Polarised Neutrons - $^3$He “cow” for all ILL  
   E. Lelievre-Berna et al. with DPT

5. High Pressure Cell - new 100 Mbar pressure cell for all ILL  
   N. Kernavanois et al. with DPT

   T. Forsyth et al. with LSS

7. All with only 2 scientists/inst - We are short of scientists
SNS Competition - Build on Our Strengths (BOOST)

1. Higher flux on the sample with CW on reactors
   - $\Delta \lambda / \lambda \gg \Delta d / d$. Flux on the sample is much higher than for TOF
   - But TOF capable of very high resolution in backscattering

2. Larger focussing monochromators, especially Ge
   - Often doubly focussing
   - Perhaps cooled for hot neutrons
   - Sometimes polarising

3. Larger 2D position sensitive detectors (D19 type)
   - For both single crystals and powders

4. Better sample environments
   - Refrigerators replacing cryostats, pressure cells, furnaces...
Why is sample flux so high from a reactor?

Large wavelength-band focusing monochromators
Focusing in reciprocal space can give a factor of $x10$

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

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Comparison of TOF & CW Diffractometers

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

With big detectors we can compete with the SNS intensity
The time-average sample flux is higher on a CW source.

<table>
<thead>
<tr>
<th></th>
<th>D20</th>
<th>GEM</th>
<th>DRACULA</th>
<th>SNS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flux average on sample</td>
<td>5x10^7</td>
<td>~2x10^6</td>
<td>~10^8</td>
<td>~2.5x10^7</td>
</tr>
<tr>
<td>Detector solid angle</td>
<td>0.27 sr</td>
<td>4.0 sr</td>
<td>1.5 sr*</td>
<td>3.0 sr</td>
</tr>
<tr>
<td>Efficiency=Flux*Detector</td>
<td>1.7</td>
<td>1</td>
<td>18</td>
<td>9</td>
</tr>
</tbody>
</table>

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

Very high flux on the sample

- D2B $1.0 \times 10^7 \text{ n.cm}^{-2}.\text{sec}^{-1}$
- D20 $9.8 \times 10^7 \text{ n.cm}^{-2}.\text{sec}^{-1}$
- IN8 $6.5 \times 10^8 \text{ n.cm}^{-2}.\text{sec}^{-1}$
Bigger Detectors
Important from the beginnings of ILL

30 years ago – D1A, D1B & D6 “Hedgehog” 1973

Original D1B PSD detector

Original D1A mono-detector

D6 single crystal hedgehog

First D1A multi-detector
20 years ago

Bigger Detectors
The Past
The ILL “No Compromise, Unique-in-the-World” decade

- No follow up on D19 detector success (No D9,D16)
- Contracting out of ILL detectors - CERCA failure
- Multiple attempts to build D20 over 15 years!
- ILL detector RESEARCH successes - microstrips...
- Loss of ILL ability to provide large PSD detectors

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Finally, after 15 years

1997
D20 Works!

1998
D20 Fails!

2000
D20 Rebuild!
Bigger Detectors
Today

New D20–2002
High flux option

Before and After (data in 2 min.)

New D20–2003
High resolution option

Higher D20 resolution since 2003
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Bigger Detectors
Today

New D2B-2003
Very High Res.

1st 2D detector
For Neutron PD

Integrate over
Diffraction Cones
Bigger Detectors
Today

New VIVALDI-2002
"As Powerful as Powders"
G. McIntyre
Bigger Detectors
The Future

New D19-2004
The Future for ILL
DRACULA, D9, D16

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Better Sample Environments

Refrigerators, Furnaces, Cryomagnets & Pressure Cells

Pulsed-Tube Refrigerator
Diffraction replacing ILL cryostats

10 Tesla D3 Cryomagnet
DifMag 7T ordered (E. Suard)

High Pressure Paris-Edin Cell
100 Kbar cell (N. Kernavanois)

Microwave Furnace
H. Boysen et al.
Polarised Neutrons

More diffraction experiments could benefit...

- $^3$He filter
- CryoPol
- Supermirror Polarisers
- Heusler Monochromators

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Hot Source Machines

- **D3**
  - Complex magnetic structures, spin, polarised neutrons.
  - \(^3\text{He},\) Cryopol, focusing mono
  - Expand the user base!

- **D4 (50%)**
  - Liquids & amorphous structures.
  - Extreme P-T, levitating furn.
  - 100% instrument in future?

- **D9**
  - High-resolution of atomic structures, complements D3.
  - Cooled monochromator?
  - A large 2D PSD detector?
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- **Thermal Instruments**
  (Same beam tube H11)
  - D19 (single crystals)
    - Chemical & Biological structures
    - More complex H-D problems
    - P-T-Humidity environments
  - D2B (high res.powder)
    - Precise Inorganic structures
    - Smaller samples, P-T-H scans
    - New 7Tesla cryomagnet
  - D20 (high int.powder)
    - Good-resolution, small samples
    - Fast P-T-H scans, kinetics
    - Radial collimation, polarised n.
Only 1 Thermal Beam for Diffraction

D5 was also thermal but taken for 2\textsuperscript{nd} C.S.

8 Thermal Beams + Thermal Guides
Publications on ILL Thermal Beam-Tubes from ILL WWW pages

Number of Papers (1999-2004)

- H6+7 (GAMS) 12
- H9  (PN1) 14
- H10 (IN8) 61
- H12 (IN4) 22
- H13 (IN20) 69
- Total 178

Only 1 Thermal Beam for Diffraction

Source: ILL library
Publications on ILL Thermal Beam-Tubes from ILL WWW pages

Only 1 Thermal Beam for Diffraction


- H6+7 (GAMS) 5
- H9 (PN1) 4
- H10 (IN8) 20
- H12 (IN4) 2
- H13 (IN20) 14
- Total 45
- H11 (D2B,D19,D20) 115

Source: ILL library
Highly cited ILL neutron diffraction papers
http://www.ill.fr/dif/citations/

Top ILL papers - Large number of citations for ILL neutron diffraction work


- **319 (D2B)** Radaelli PG, Cox DE, Marezio M, Cheong, SW (1997) *Phys.Rev.* B55, 3015. Charge, orbital, and magnetic ordering in La(0.5)Ca(0.5)MnO3.
Only 1 Thermal Guide for Diffraction (H22) + D10

- D1A
- D1B
- SALSA
- VIVALDI

Proposed H112 (LADI3, IN16B)

H112 would kill D1A (BRITTAX), block VIVALDI access and prevent further development of new H22 SM-guide
Diffraction Deserves a 2nd Thermal Beam

DRAC, first presented at the ILL “Instrument Day” 26 Feb 2002
DRAC, highest priority for Instrument Committee 17 Oct 2003
Instrument Subcommittee October 4th, 2004

DRACULA - Summary and Recommendations - D. Richter, Chairman.

1. **Unique ability to focus away from back-scattering**
   Unique instruments, little competition from pulsed sources.

2. **Collecting many wavelengths near the focussing point**
   Opens very exciting opportunities... eg high-pressure research.

3. **DRACULA would be unsurpassed with respect to intensity**
   Given the present planning for instrumentation at SNS.

4. **The conflict between the Neutro-Graph and DRACULA concerning H9 needs to be resolved...**
DRACULA on Thermal Beam Tube H9
Co-existence of DRACULA & Tomography
What is ILL’s Mission, How is it Changing...?

1. **Unique-In-The-World facilities?** No longer true...
   ILL flux no longer x10 greater, others have good machines

2. **Inventing New Techniques?** Never really true...
   Medium flux sources have more spare time, more students...

3. **World’s Best Instruments?** Yes – even with American SNS
   Provided we BOOST – high sample flux, detectors, sample environment

4. **Unique Research Culture?** Yes – ESRF, EMBL, IBS, PSB...
   A European meeting place for people, science & technology
ILL’s Future

How do we become more relevant to our clients?

1. We must listen to what they want.
   They need to publish, train students, teach & exchange experience

2. We should involve them in our projects.
   Projects like D2B, D19, SALSA, Fame38, D-Lab...
   June 2005, ILL Conference, Progress with EPSRC Millennium projects

3. Projects more relevant to a wider user community.
   Fewer “Unique-in-World” projects aimed at neutron “professionals”

4. Define **measures of success** for projects
   Time scales, budgets, numbers of users, proposals, papers, citations...

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Thank you...

To the Science Council for Listening...
To Ted Forgan, for asking the right questions...
And all the members of the ILL Diffraction Group
Who helped me to answer them...