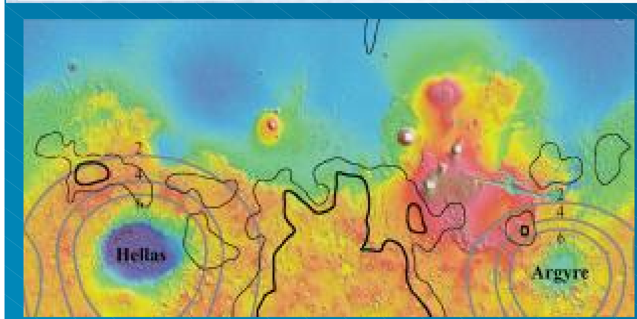
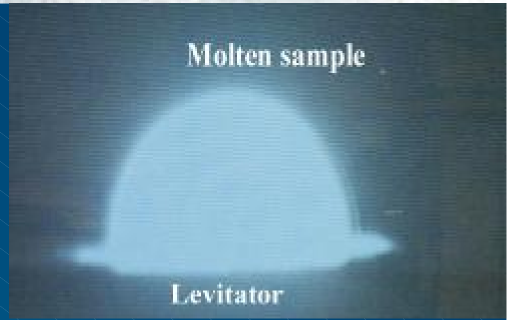
The ILL Diffraction Group

The ILL Diffraction Group

Alan Hewat, Diffraction Group Leader



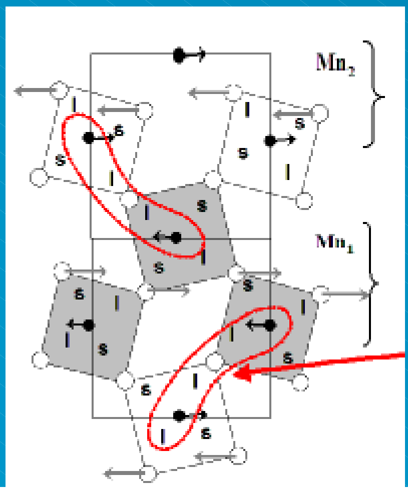
- Magnetism on Mars



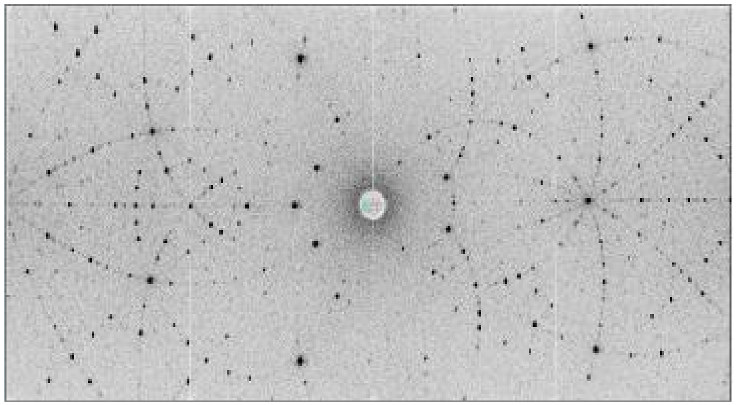
- Levitation at 3000ºC

- Polymer Structures

- Polarised Eddies



- Zener Polarons



- Reciprocal Space Explorer

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...)*

Where are we now ?
Where are we going ?

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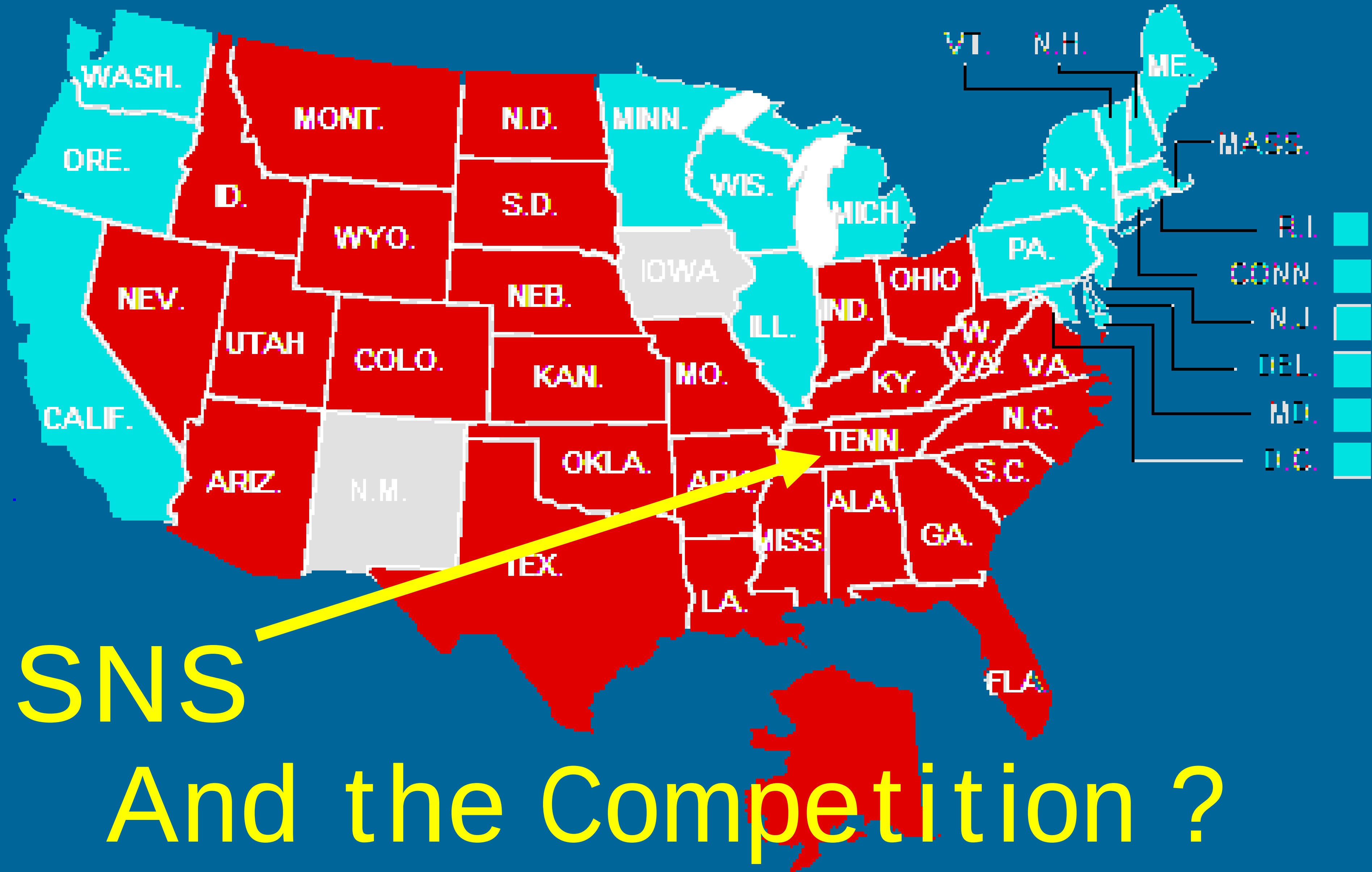
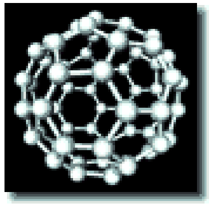


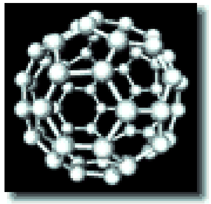
SNS

And the Competition ?



ILL Diffraction instruments can be divided into 3 groups:

- *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.
- *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.
- *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:

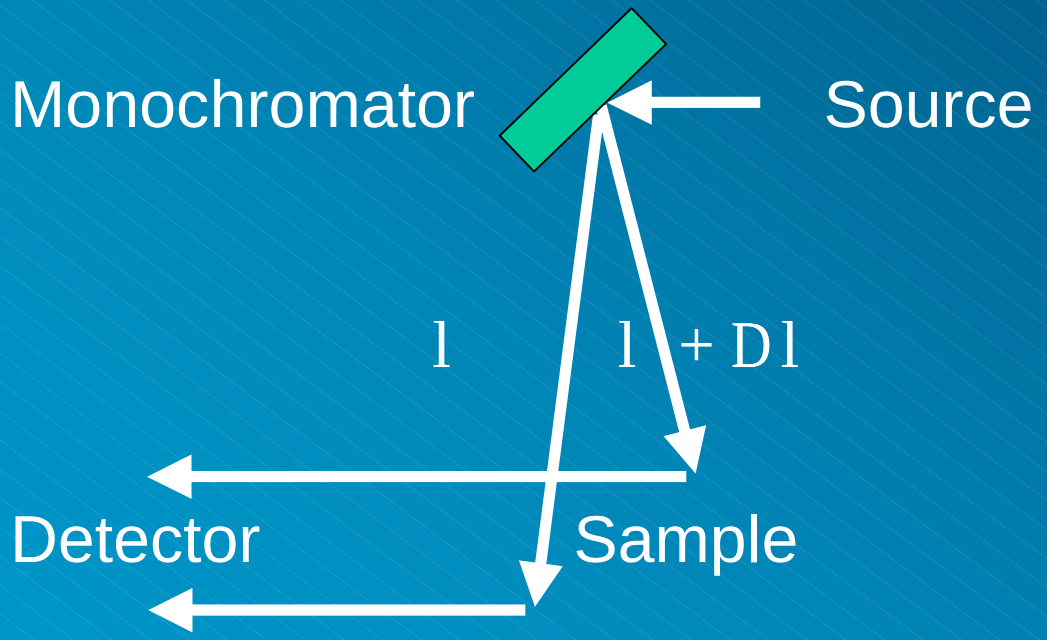
- *SALSA strain scanner – new EPSRC financed project*
  Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)
- *FaME38 Engineering Lab.– new EPSRC financed project*
  P. Webster et al. (Salford)
- *Crystal Alignment Machine – new test machine for all ILL*
  B. Ouladdiaf
- *^{3}He cell for Polarised Neutrons – ^{3}He "cow" for all ILL*
  E. Lelievre-Berna et al. with DPT
- *High Pressure Cell – new 100 Mbar pressure cell for all ILL*
  N. Kernavanois et al. with DPT
- *Support for Deuteration lab.*
  T. Forsyth et al. with LSS
- *All with only 2 scientists/inst - We are short of scientists*

SNS Competition - Build on Our Strengths (BOOST)

- *Higher flux on the sample with CW on reactors*
  - $\Delta\lambda/\lambda >> \Delta d/d$. Flux on the sample is much higher than for TOF
  - But TOF capable of very high resolution in backscattering
- *Larger focussing monochromators, especially Ge*
  - Often doubly focussing
  - Perhaps cooled for hot neutrons
  - Sometimes polarising
- *Larger 2D position sensitive detectors (D19 type)*
  - For both single crystals and powders
- *Better sample environments*
  - Refrigerators replacing cryostats, pressure cells, furnaces…

Large wavelength-band focusing monochromators

Focusing in reciprocal space can give a factor of x10



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

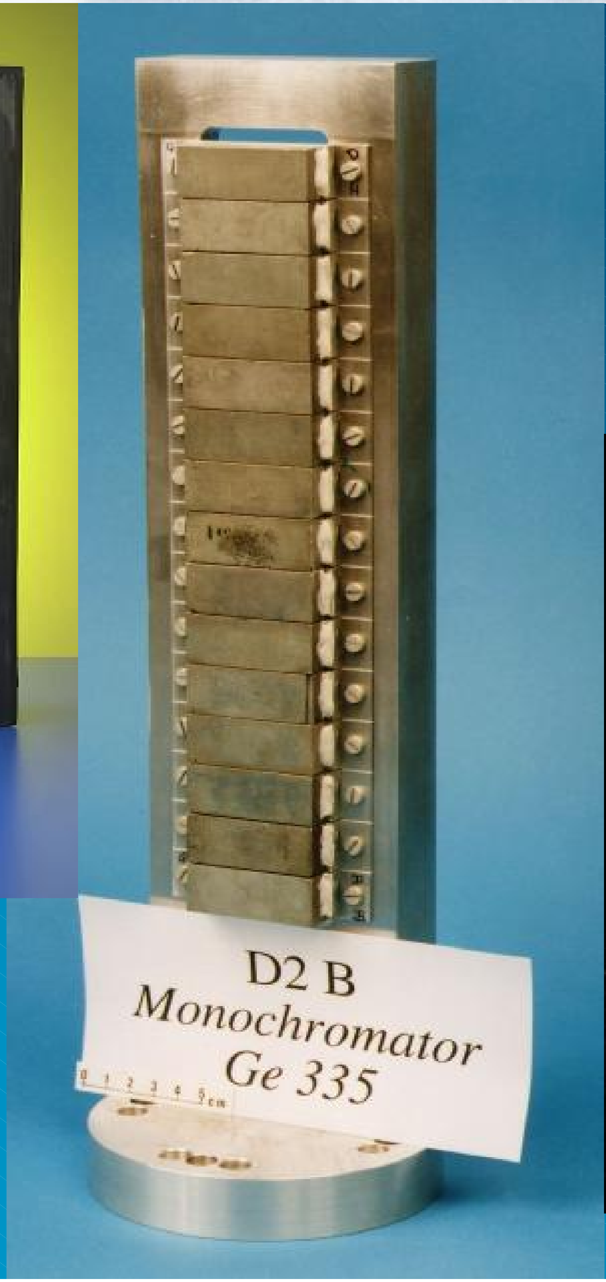
The time-averaged Flux*Detector criterium

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

	D20	GEM	DRACULA	SNS
Flux average on sample	5×10^7	$\sim 2 \times 10^6$	$\sim 10^8$	$\sim 2.5 \times 10^7$
Detector solid angle	0.27 sr	4.0 sr	1.5 sr*	3.0 sr
Efficiency=Flux*Detector	1.7	1	18	9

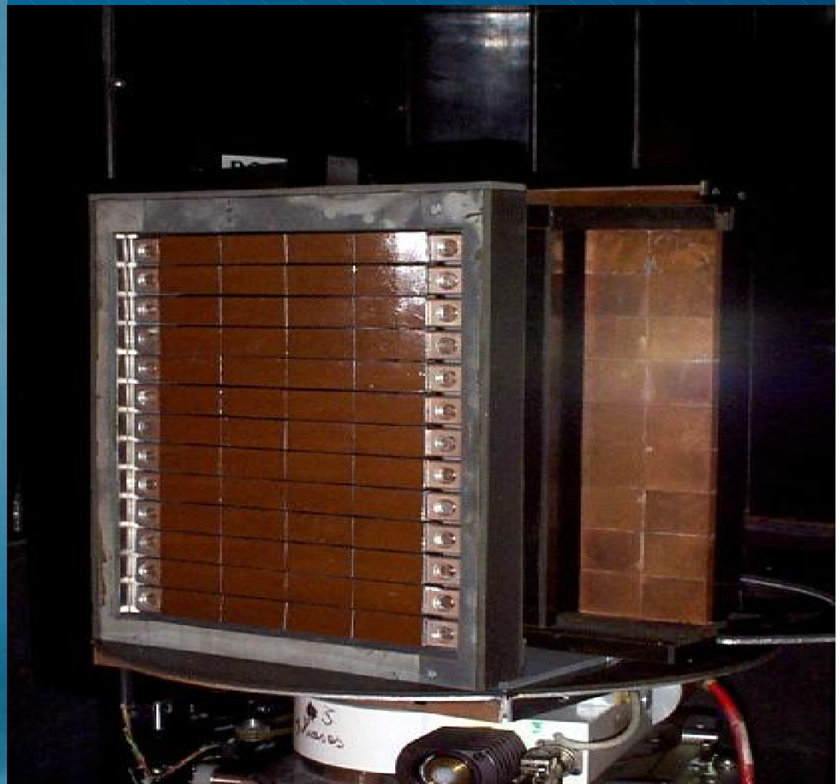
* Based on new D19 detector: R=760 mm, h=400 mm, 800 linear resistive wires 30°x160°

Better monochromators



Very high flux on the sample

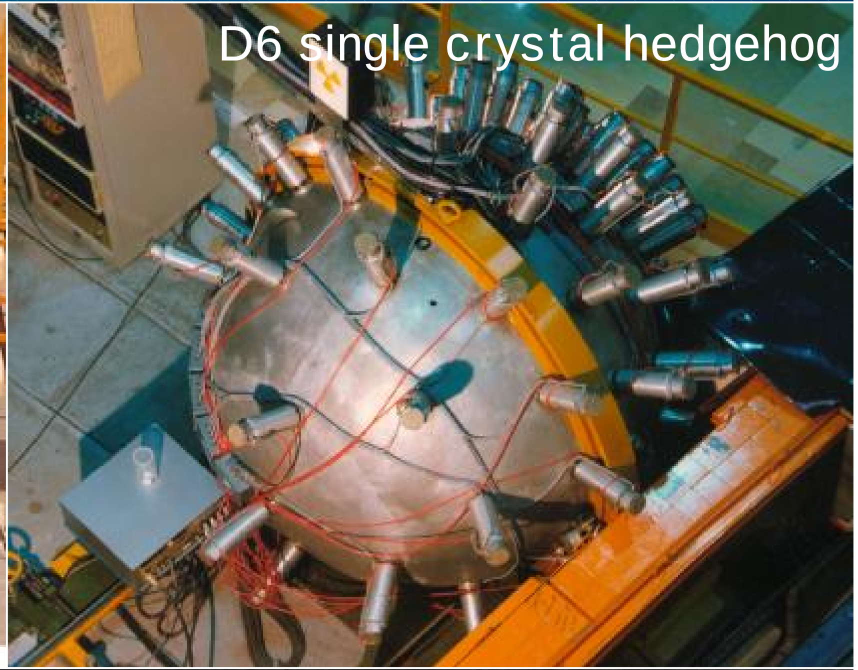
- D2B 1.0×10^{7} $n.cm^{-2}.sec^{-1}$
- D20 9.8×10^{7} $n.cm^{-2}.sec^{-1}$
- IN8 6.5×10^{8} $n.cm^{-2}.sec^{-1}$



Bigger Detectors
Important from the beginnings of ILL

30 years ago – D1A, D1B & D6 "Hedgehog" 1973

Original D1B PSD detector



D6 single crystal hedgehog

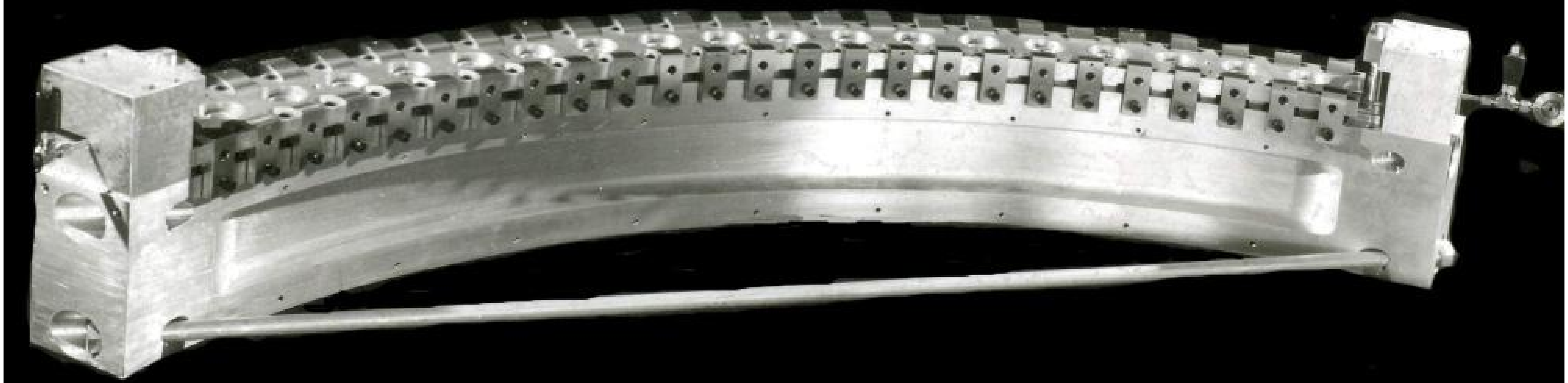
Original D1A mono-detector

First D1A multi-detector

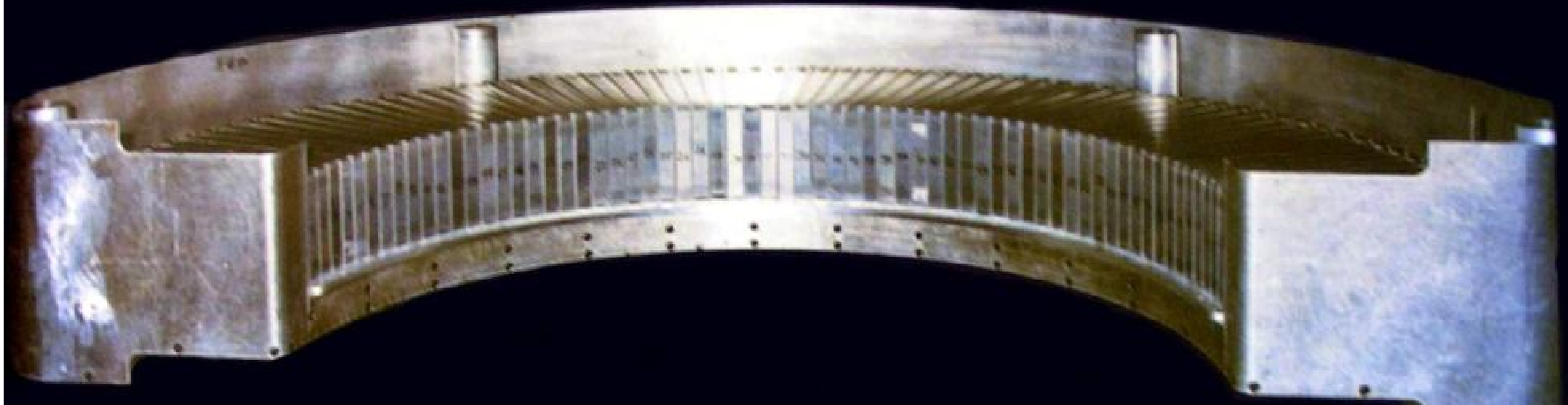
Bigger Detectors
The Past

20 years ago

D19-1983



D2B-1983



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

Bigger Detectors
The Past

Finally, after 15 years

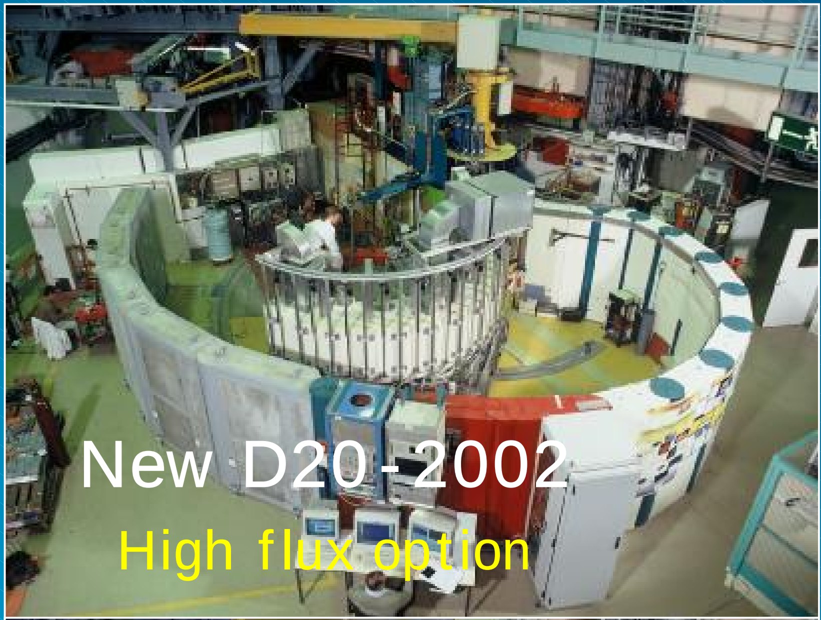
1997
D20 Works !

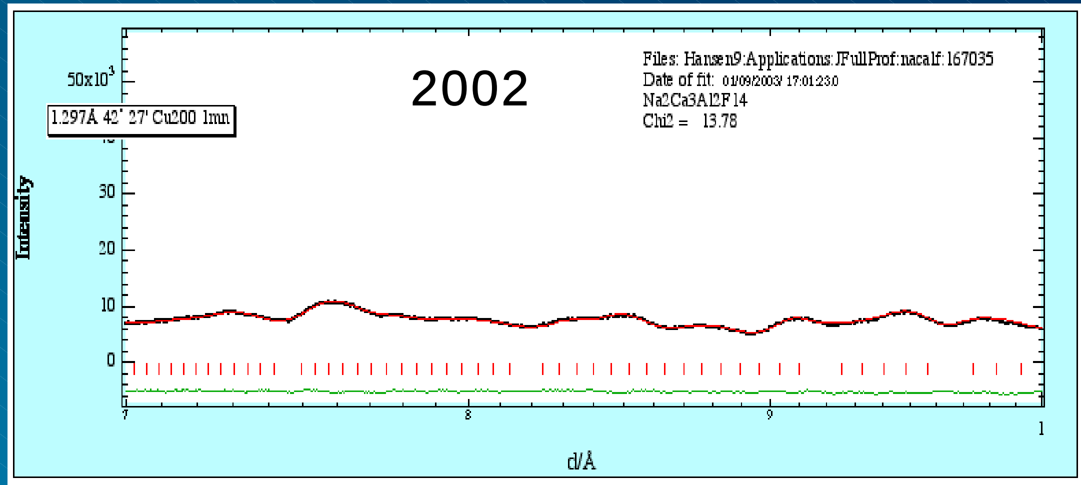
1998
D20 Fails !

2000
D20 Rebuild !

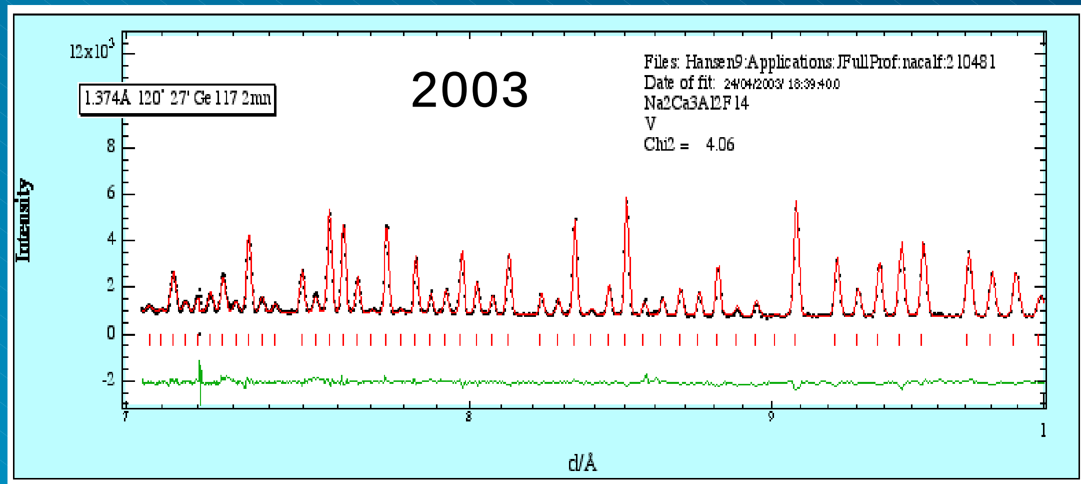
p://www.ill.fr/dif/AlanHewat/

Bigger Detectors Today





Before and After (data in 2 min.)



Higher D20 resolution since 2003

Bigger Detectors
Today

New D2B-2003

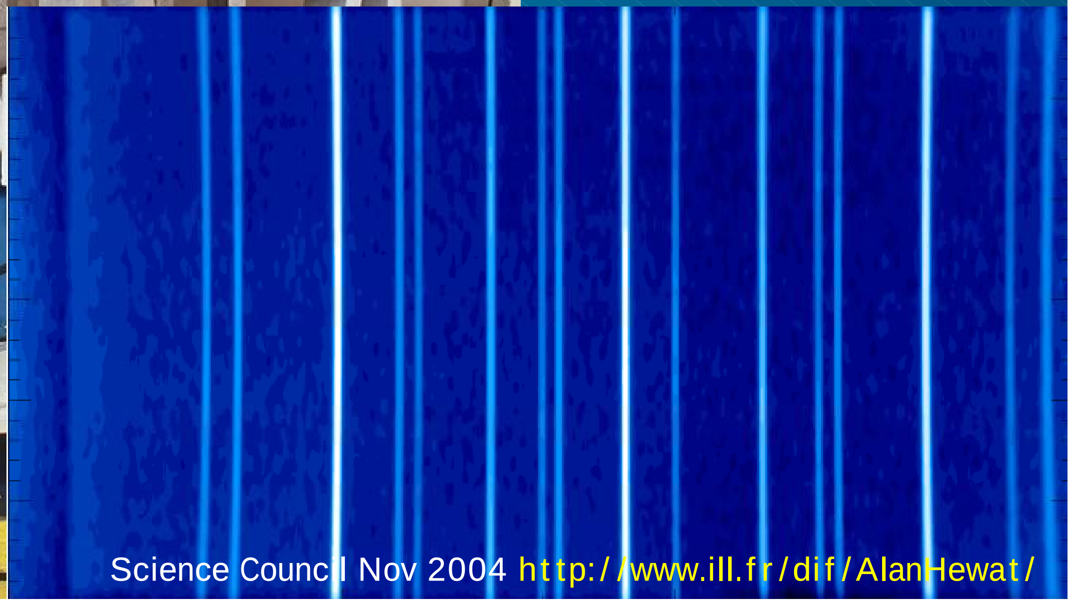
Very High Res.

1st 2D detector

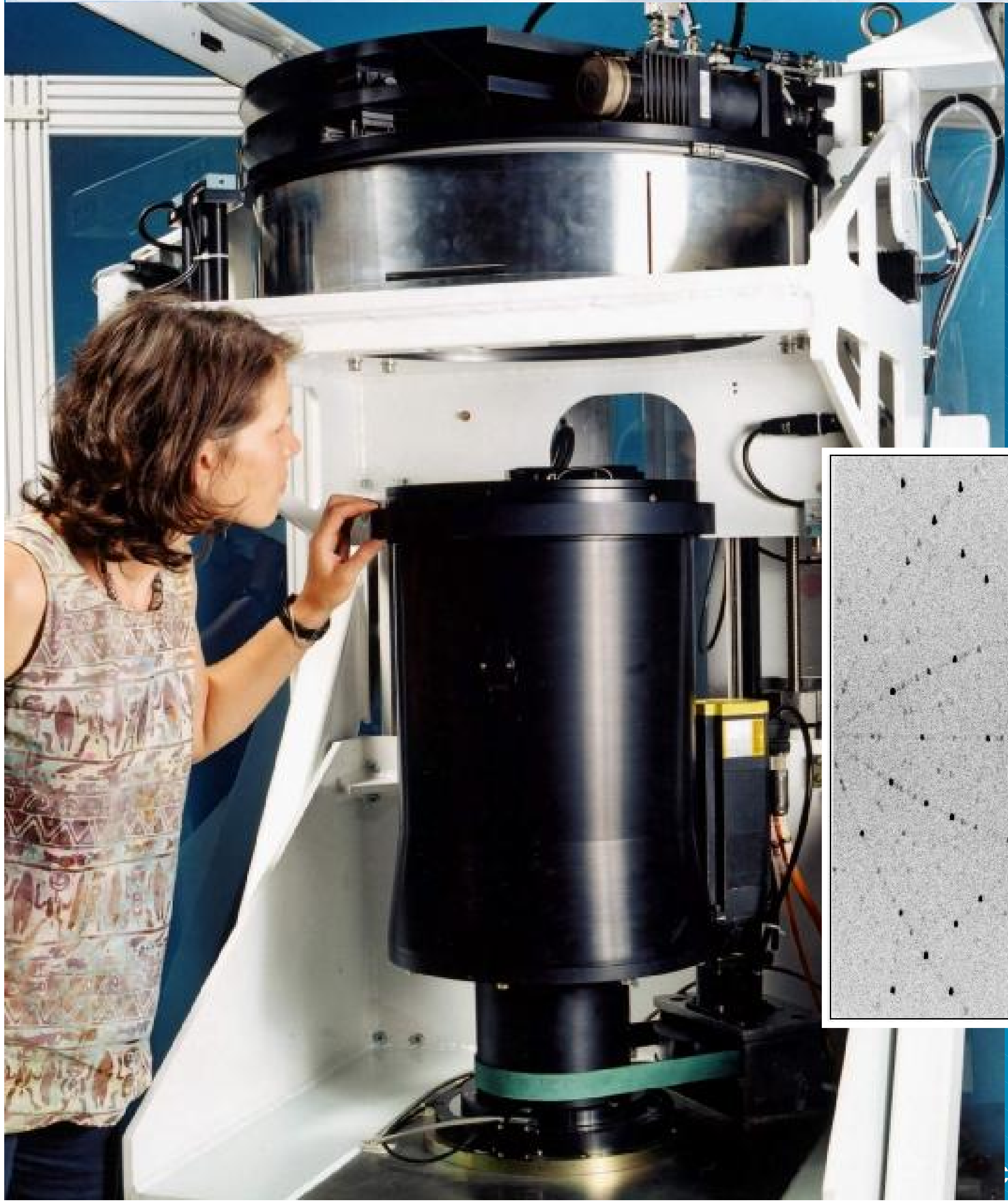
For Neutron PD

Integrate over

Diffraction Cones

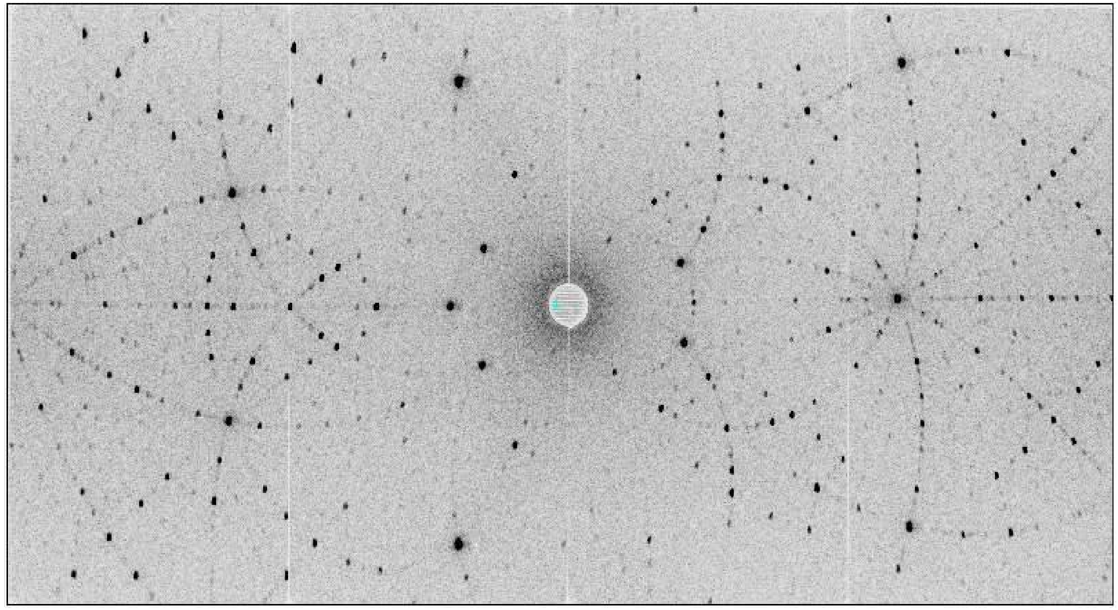


Bigger Detectors Today



New VIVALDI-2002

"As Powerful as Powders"
G. McIntyre



Bigger Detectors
The Future

New D19-2004

The Future for ILL

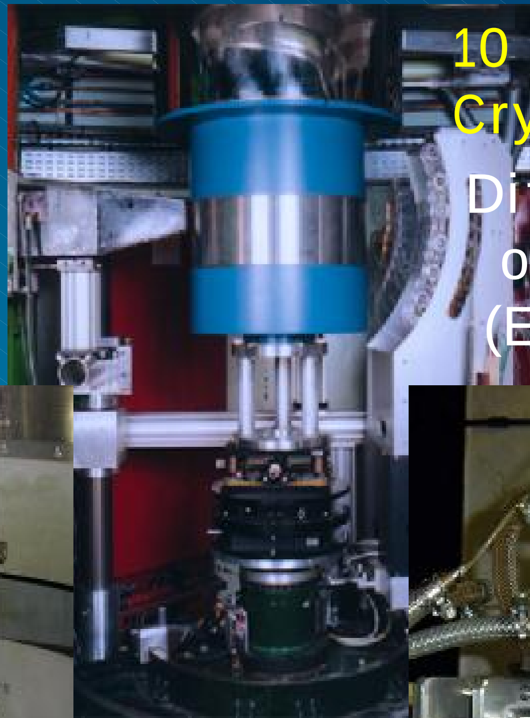
DRACULA, D9, D16

Better Sample Environments

Refrigerators, Furnaces, Cryomagnets & Pressure Cells

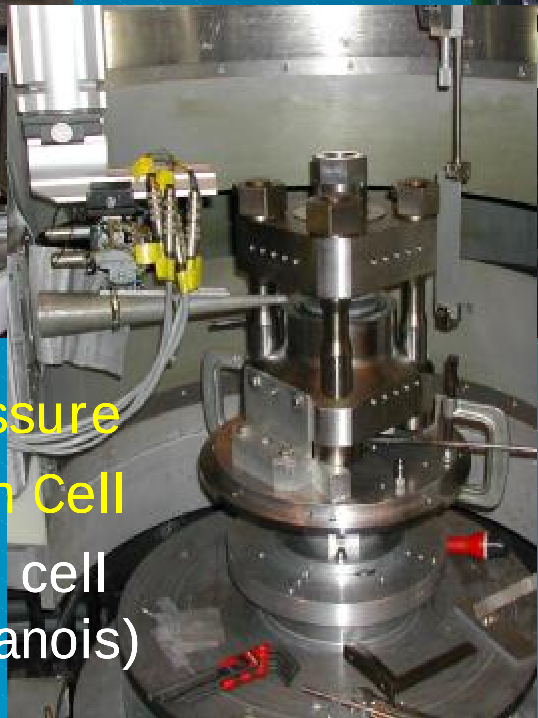
Pulsed-Tube Refrigerator

Diffraction replacing ILL cryostats



10 Tesla D3 Cryomagnet

DifMag 7T ordered (E.Suard)



High Pressure Paris-Edin Cell

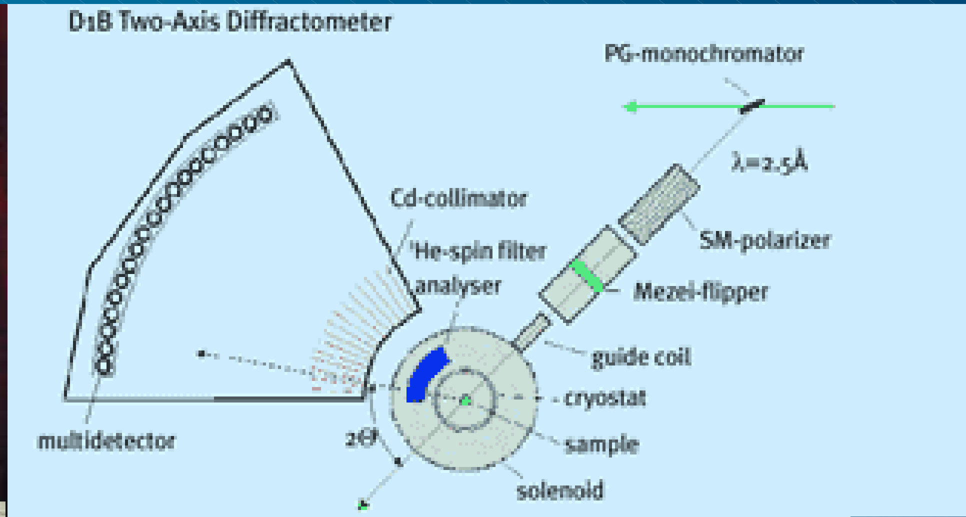
100 Kbar cell (N.Kernavanois)

Microwave Furnace

H.Boysen et al.

More diffraction experiments could benefit…

^{3}He filter

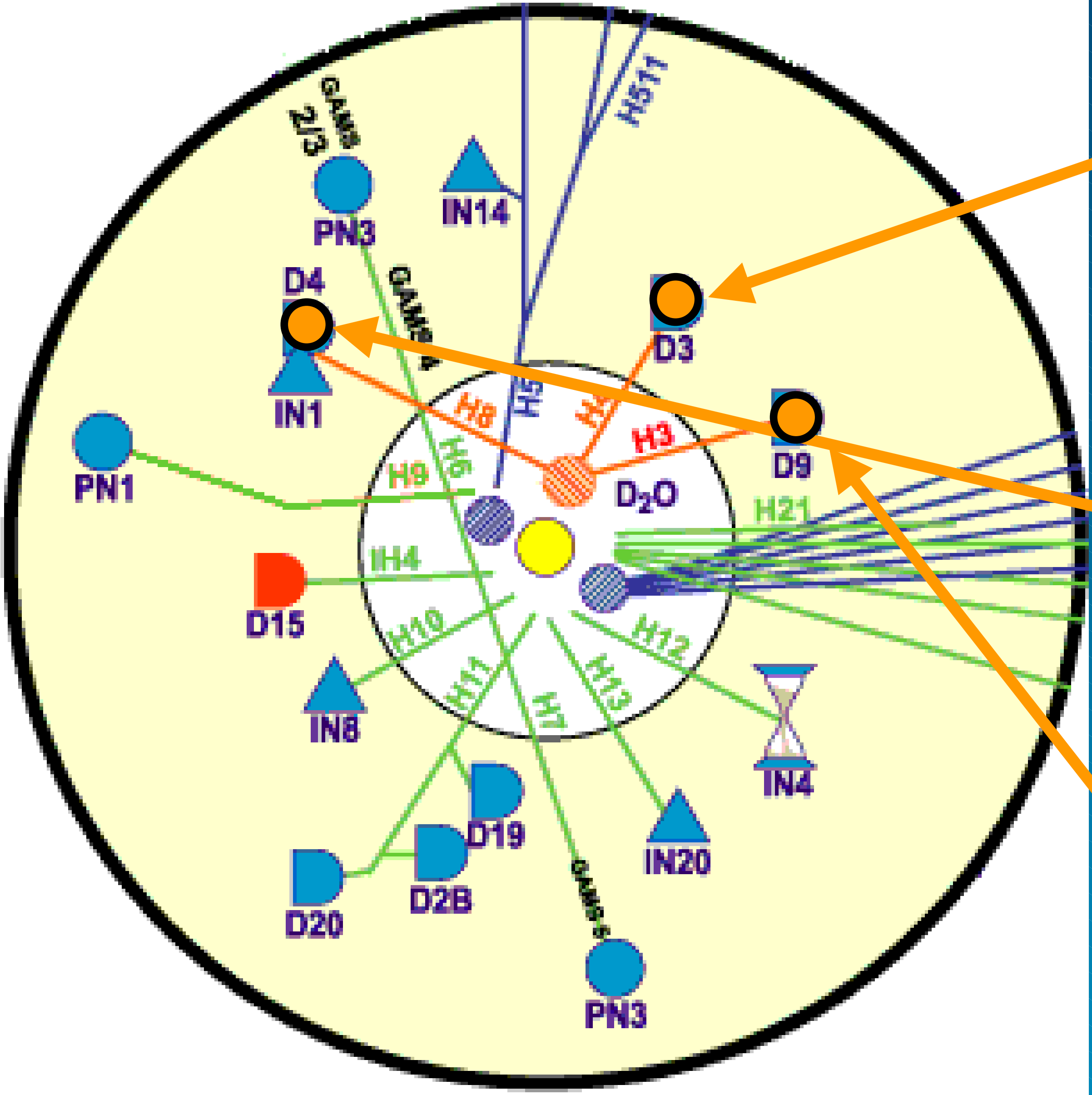


^{3}He “cow”

CryoPol

Supermirror Polarisers

Heusler Monochromators



Hot Source Machines

- **D3**
  Complex magnetic structures, spin, polarised neutrons.
  - ^{3}He, Cryopol, focussing 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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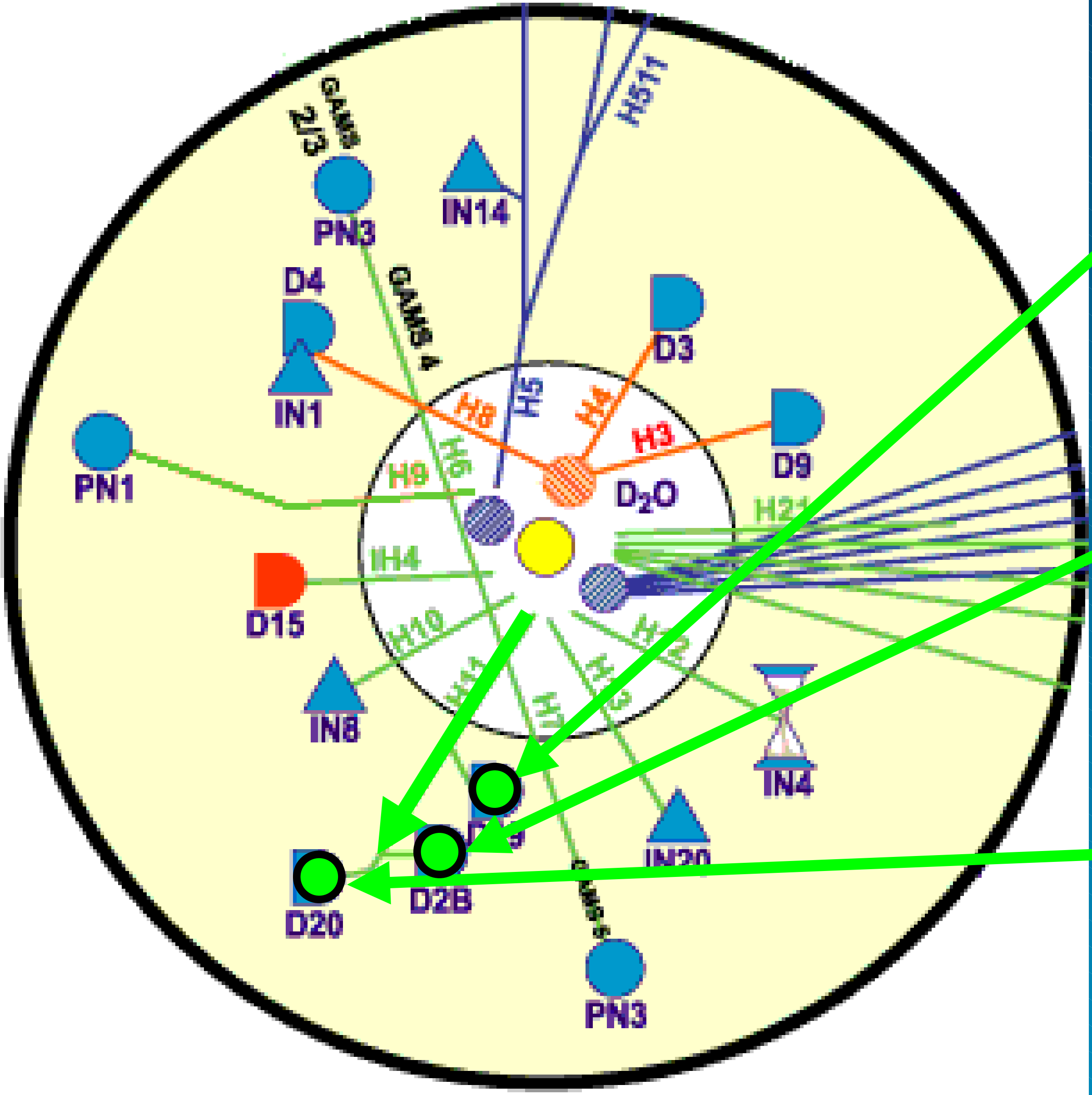
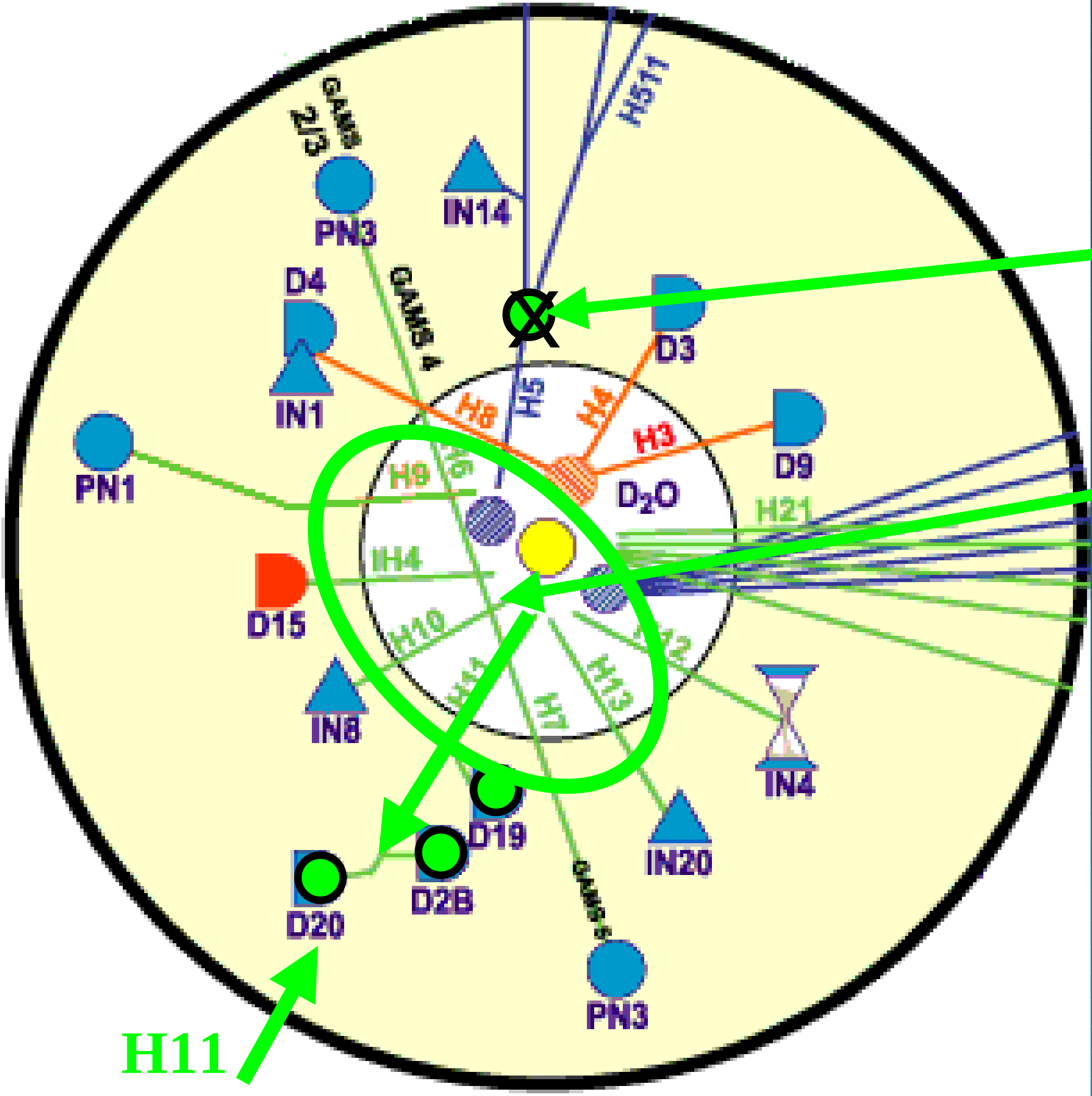


Thermal Instruments (Same beam tube H11)

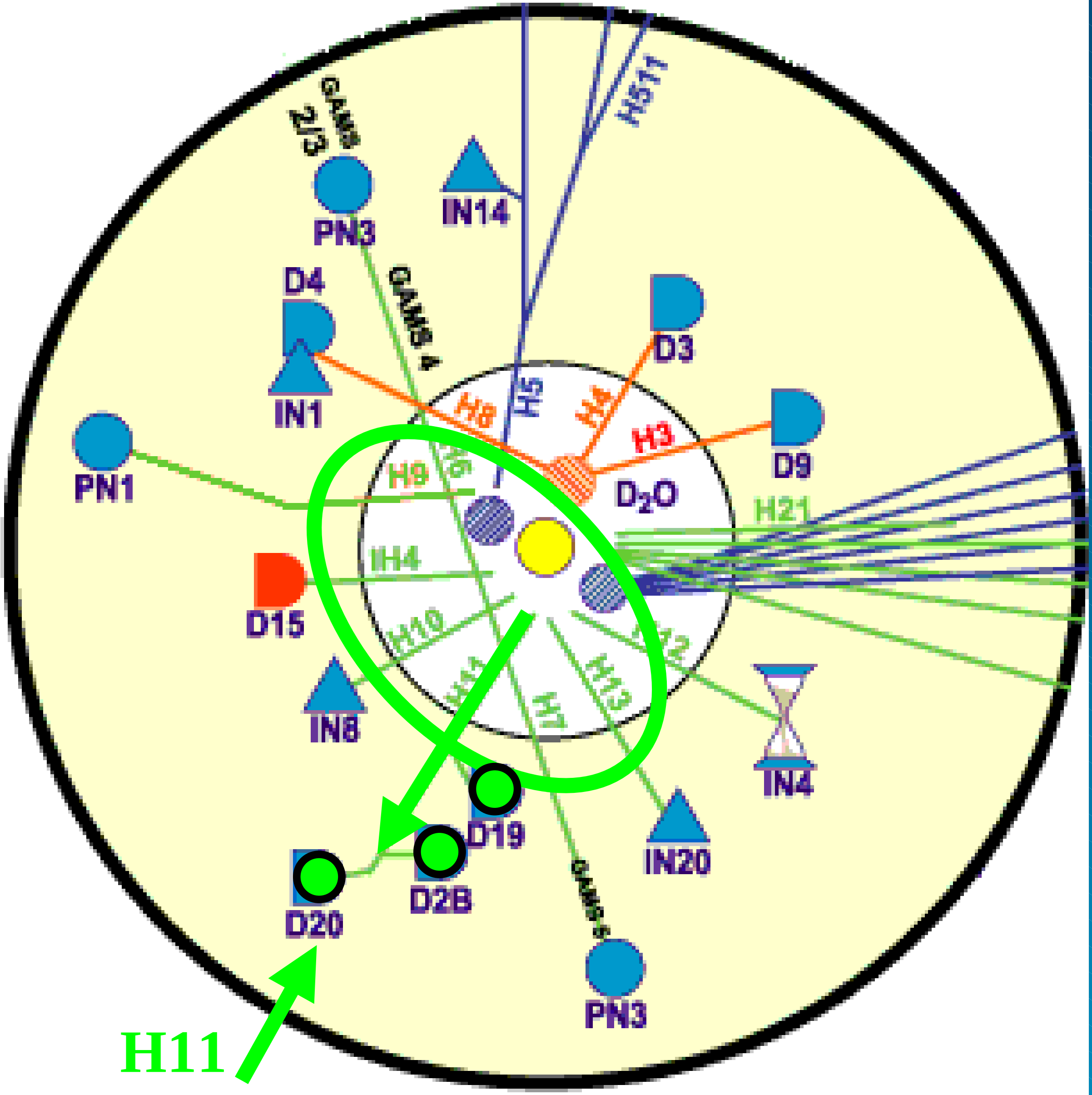
- **D19 (single crystals)**
  Chemical & Biological structures
  - More complex H-D problems
  - P-T-Humidity environments
- **D2B (high res.powder)**
  Precise Inorganic structures
  - Smaller samples, P-T-H scans
  - New 7Tesla cryomagnet
- **D20 (high int.powder)**
  Good-resolution, small samples
  - Fast P-T-H scans, kinetics
  - Radial collimation, polarised n.



Only 1 Thermal Beam for Diffraction

- D5 was also thermal but taken for 2nd C.S.
- 8 Thermal Beams + Thermal Guides

Publications on ILL Thermal Beam-Tubes from ILL WWW pages



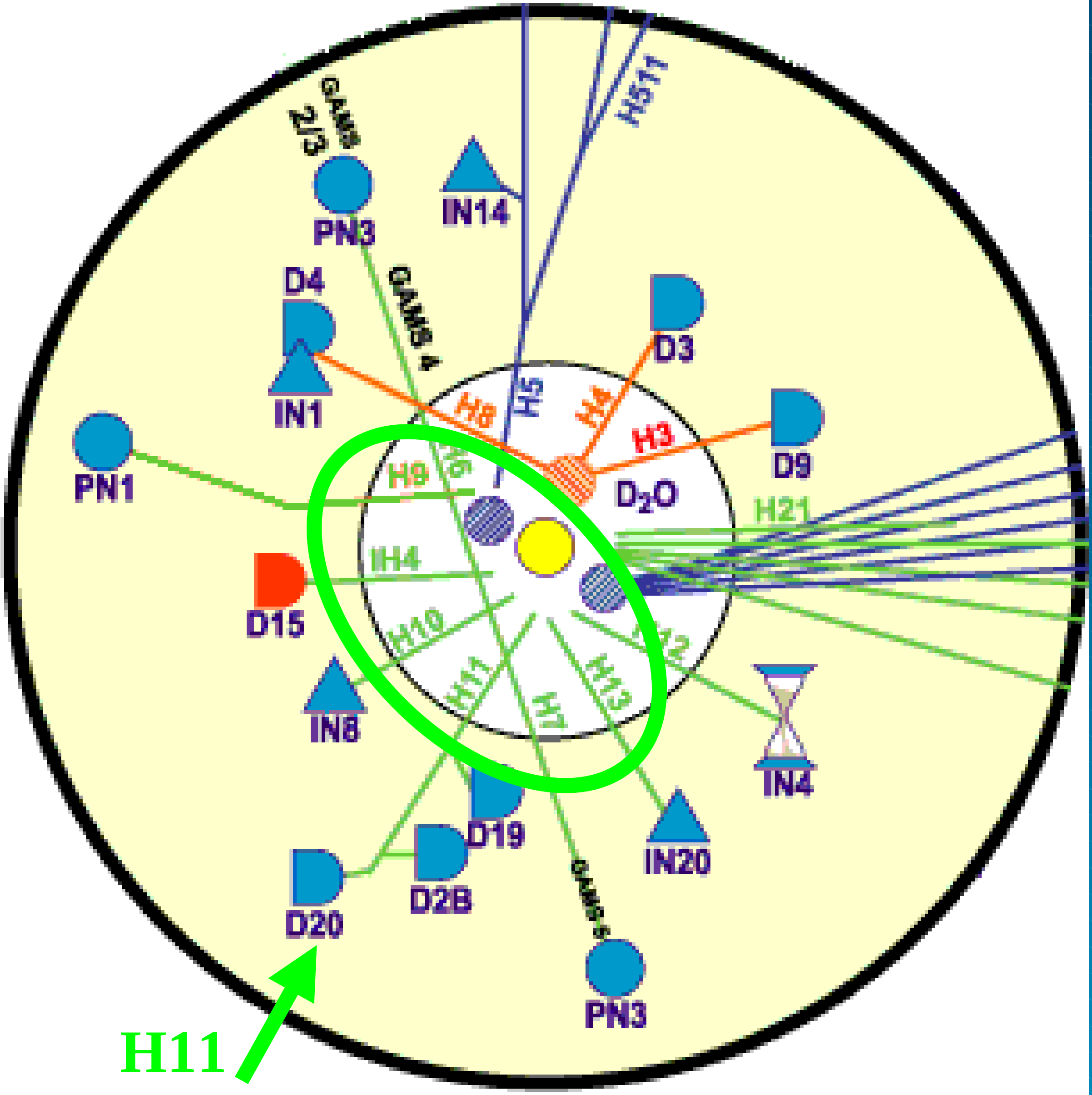
Only 1 Thermal Beam for Diffraction

Number of Papers (1999-2004)

H6+7 (GAMS)	12
H9 (PN1)	14
H10 (IN8)	61
H12 (IN4)	22
H13 (IN20)	69
Total	178
H11 (D2B,D19,D20)	458

Source: ILL library

Publications on ILL Thermal Beam-Tubes from ILL WWW pages

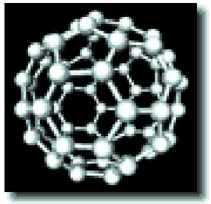


Only 1 Thermal Beam for Diffraction

PRL, Phys.Rev., JACS, Nature, Science (1999-2004)

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

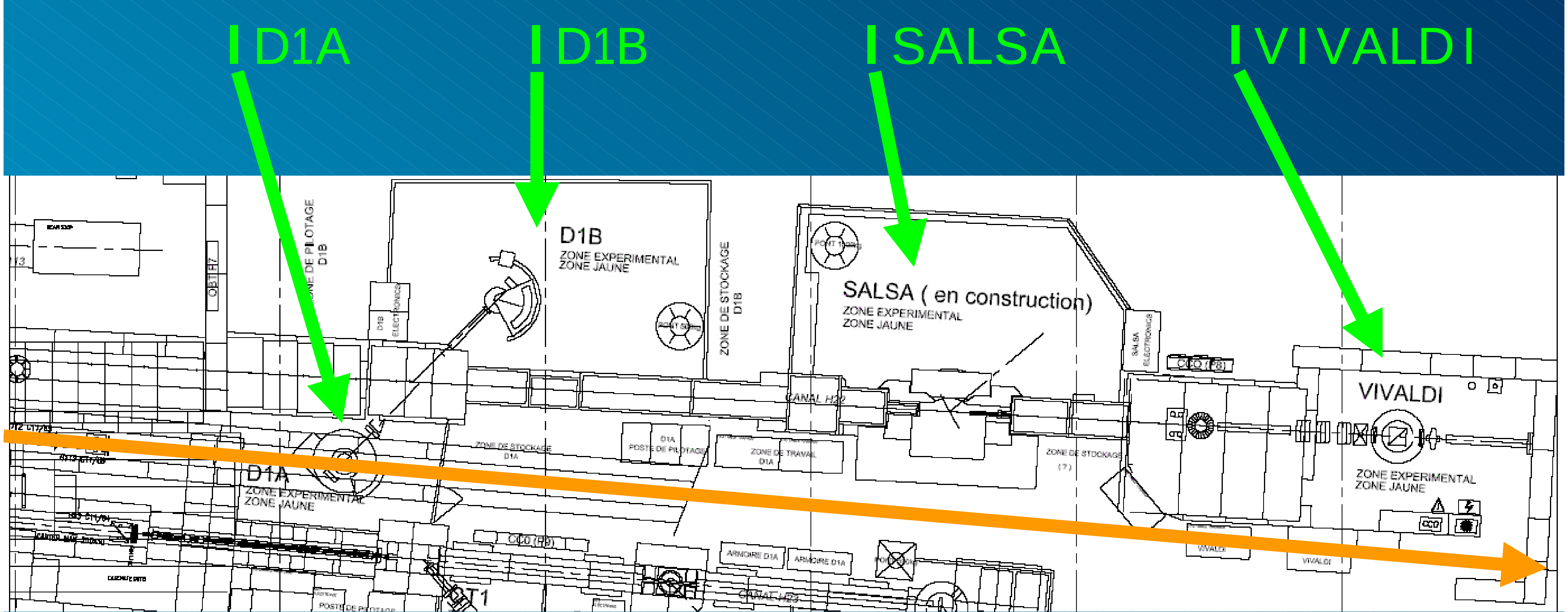
http://www.ill.fr/dif/citations/

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

- **922 (D2B)** Hwang HY, Cheong SW, Radaelli PG, Marezio M, Batlogg B (1995) **Phys.Rev.Lett. 75**, 914.
Lattice effects on the magnetoresistance in doped LaMnO3.
- **856 (D2B)** Cava RJ, Hewat AW, Hewat EA, Batlogg B, Marezio M, Rabe KM, Krajewski JJ, Peck WF, Rupp LW (1990) **Physica C. 165**, 419.
Structural anomalies oxygen ordering and superconductivity in oxygen deficient Ba2YCu3Ox.
- **501 (D1A)** Capponi JJ, Tournier R, Chaillout C, Hewat AW, Lejay P, Marezio M, Nguyen N, Raveau B, Soubeyroux JL, Tholence JL (1987) **Europhysics Letters. 3,** 1301.
Structure of the 100K superconductor Ba2YCu3O7 between 5-300K by neutron powder diffraction.
- **435 (IN8)** Rossat-Mignod, J. M., L. P. Regnault, et al. (1991) **Physica C 185-189**: 86-92.
Neutron scattering study of the YBa2Cu3O6+x system.
- **367 (D16)** Deteresa JM, Ibarra MR, Algarabel PA, Ritter C, Marquina C, Blasco J, Garcia J, Delmoral A, Arnold Z (1997) **Nature 386,** 256-259
Evidence for magnetic polarons in the Magnetoresistive materials
- **337 (D1A)** Fitch, A. N., H. Jobic, et al. (1986). **Journal of Physical Chemistry 90**, 1311-1318
Localization of benzene in sodium-Y, zeolite by powder neutron diffraction.
- **335 (IN6)** Buchenau, U., M. Prager, et al. (1986). **Physical Review B 34**, 5665-5673.
Low-Frequency modes in vitreous silica.
- **332 (IN13)** Doster, W., S. Cusack, et al. (1989) **Nature 337**: 754-756.
Dynamical transition of myoglobin revealed by inelastic neutron scattering.
- **321 (D2B)** Radaelli PG, Cox DE, Marezio M, Cheong SW, Schiffer PE, Ramirez AP (1995) **Phys.Rev.Lett. 75,** 4488
Simultaneous structural, magnetic, and electronic-transitions in La(1-x)Ca(x)MnO3 with x=0.25 and 0,5
- **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

Diffractometer for
Rapid
Acquisition over
Ultra
Large
Areas

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

DRAC, highest priority for Instrument Committee 17 Oct 2003

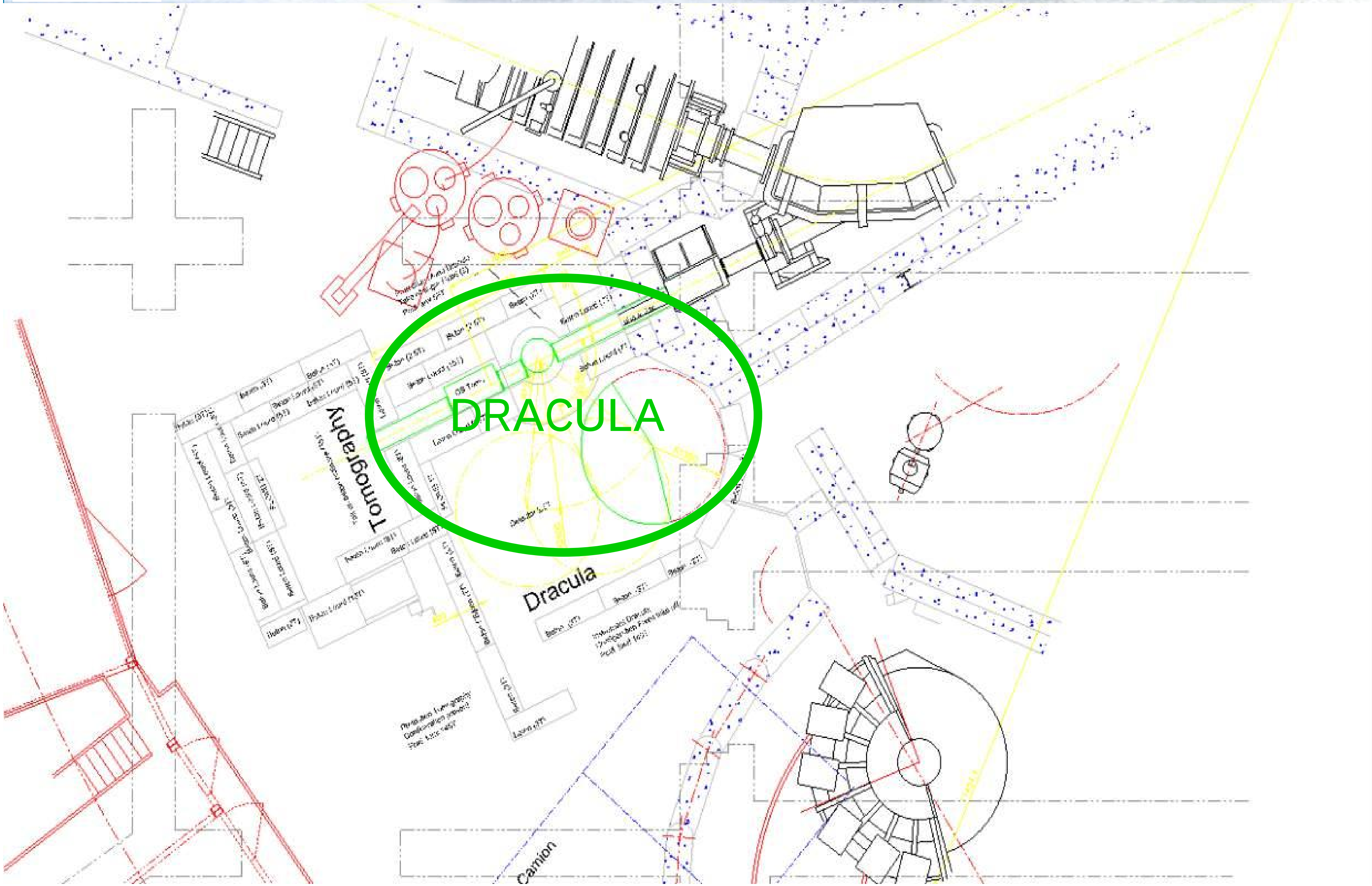
DRACULA on Thermal Beam Tube H9
Co-existance of DRACULA & Tomography

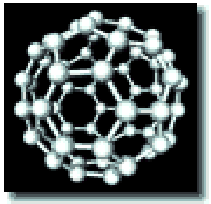
Instrument Subcommittee October 4th, 2004

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

- **Unique ability to focus away from back-scattering**
  Unique instruments, little competition from pulsed sources.
- **Collecting many wavelengths near the focussing point**
  Opens very exciting opportunities… eg high-pressure research.
- **DRACULA would be unsurpassed with respect to intensity**
  Given the present planning for instrumentation at SNS.
- **The conflict between the Neutro-Graph and DRACULA**
  concerning H9 needs to be resolved…

DRACULA on Thermal Beam Tube H9
Co-existance of DRACULA & Tomography





ILL's Future

What is ILL's Mission, How is it Changing... ?

- **Unique-In-The-World facilities ?** No longer true...
  ILL flux no longer x10 greater, others have good machines
- **Inventing New Techniques ?** Never really true...
  Medium flux sources have more spare time, more students...
- **World's Best Instruments ?** Yes – even with American SNS
  Provided we BOOST – high sample flux, detectors, sample environment
- **Unique Research Culture ?** Yes – ESRF, EMBL, IBS, PSB...
  A European meeting place for people, science & technology

How do we become more relevant to our clients ?

- We must listen to what they want.

  They need to publish, train students, teach & exchange experience

- We should involve them in our projects.

  Projects like D2B, D19, SALSA, Fame38, D-Lab…

  June 2005, ILL Conference, Progress with EPSRC Millennium projects

- Projects more relevant to a wider user community.

  Fewer "Unique-in-World" projects aimed at neutron "professionals"

- Define <u>measures of success</u> for projects

  Time scales, budgets, numbers of users, proposals, papers, citations…

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...