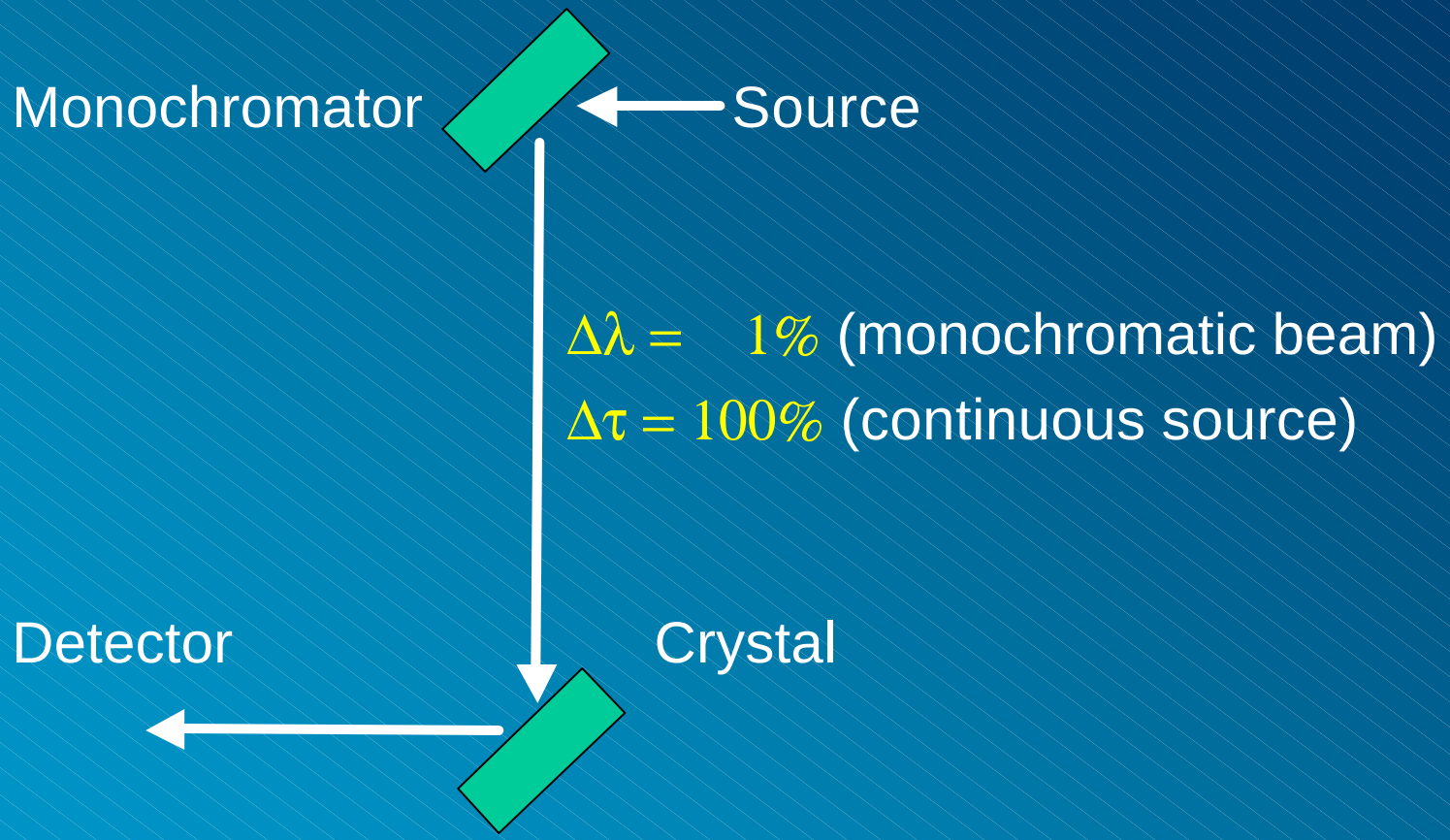
High Flux Neutron Diffractometers

Alan Hewat, ILL Grenoble

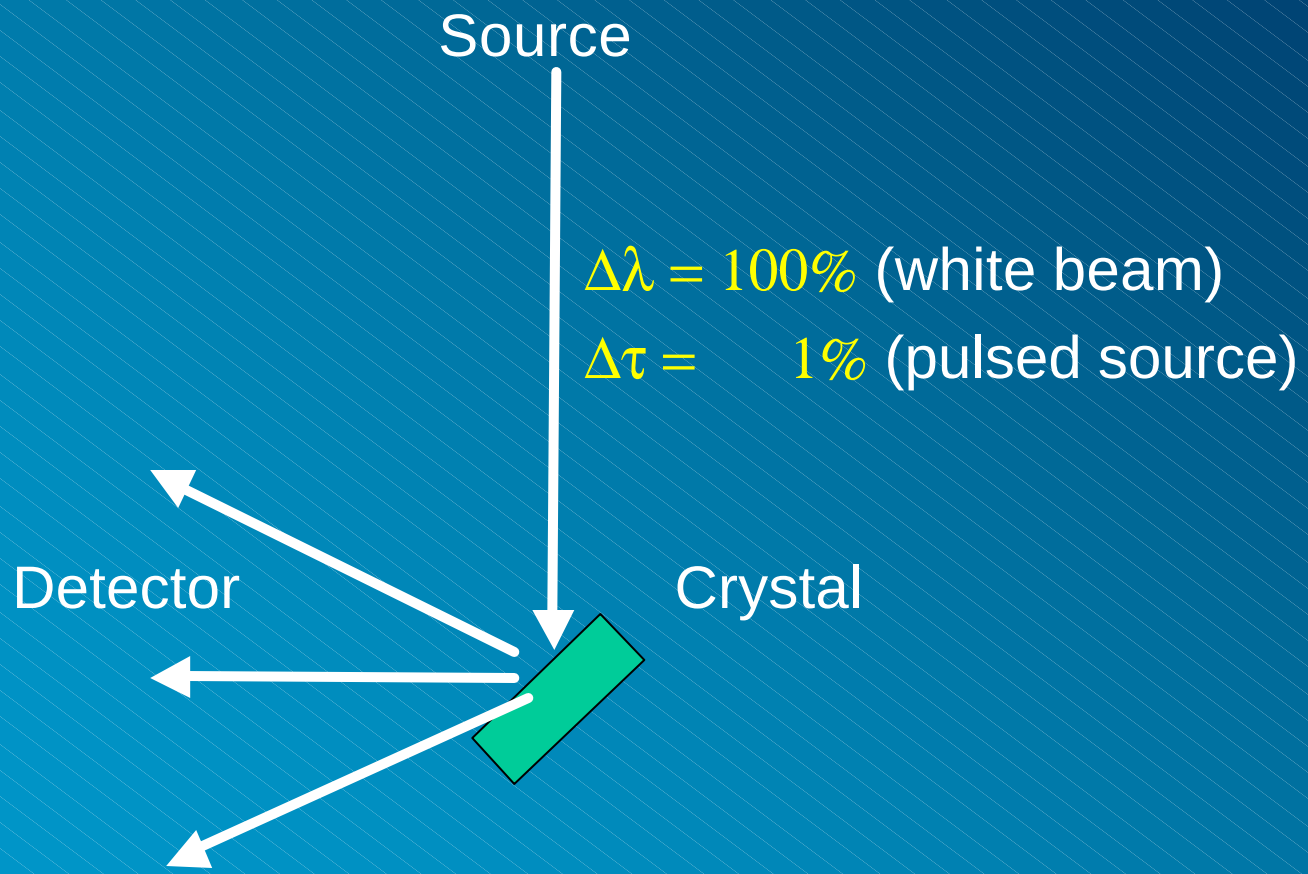
BCA Loughborough 12 April 2005

Classical Neutron Diffraction from a single crystal



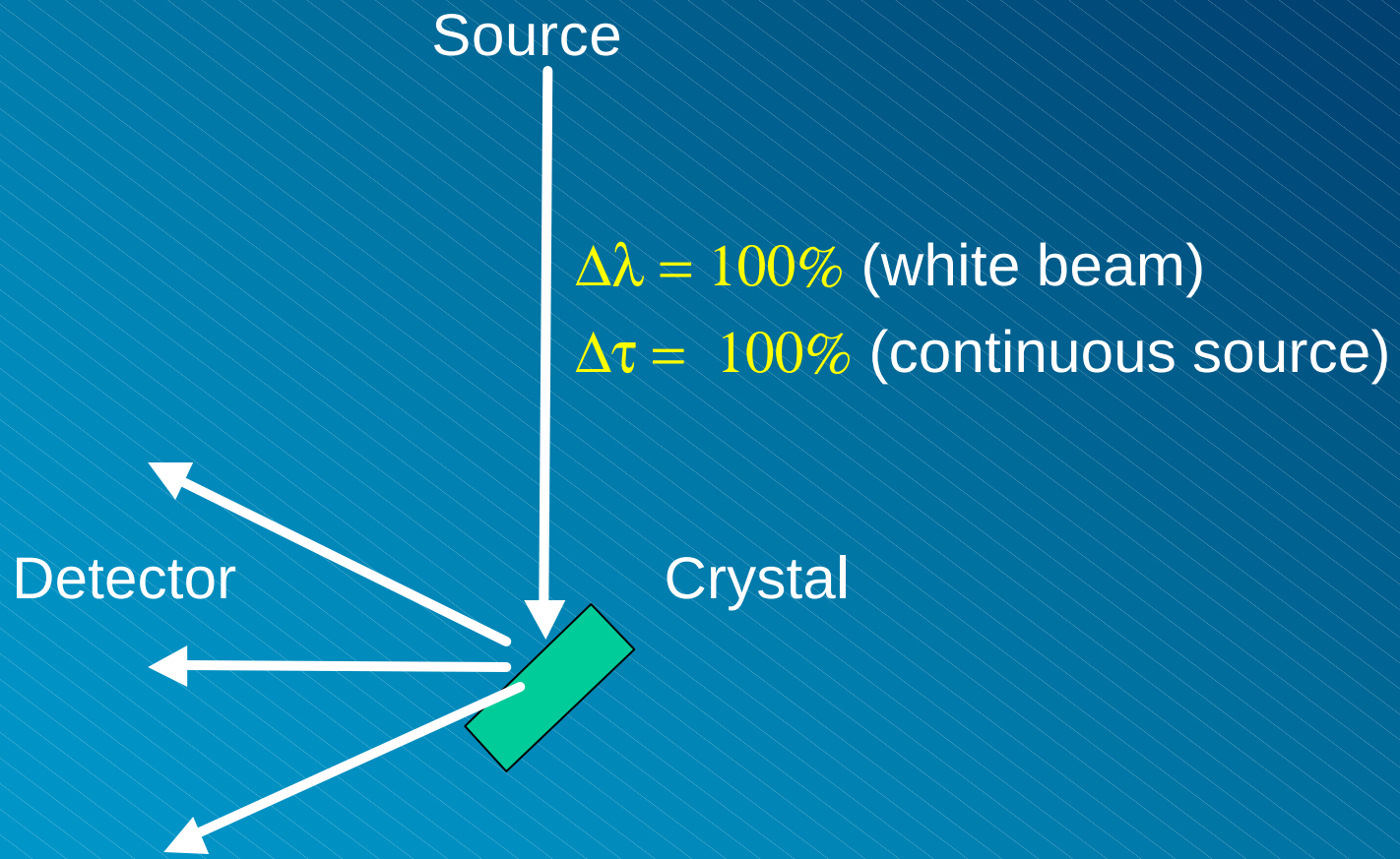
TOF Neutron Diffraction from a single crystal

Multiple reflections sorted by Time-Of-Flight



White Beam Neutron Diffraction from a single crystal

Multiple reflections sorted by the Crystal itself



High Flux Neutron Diffractometers

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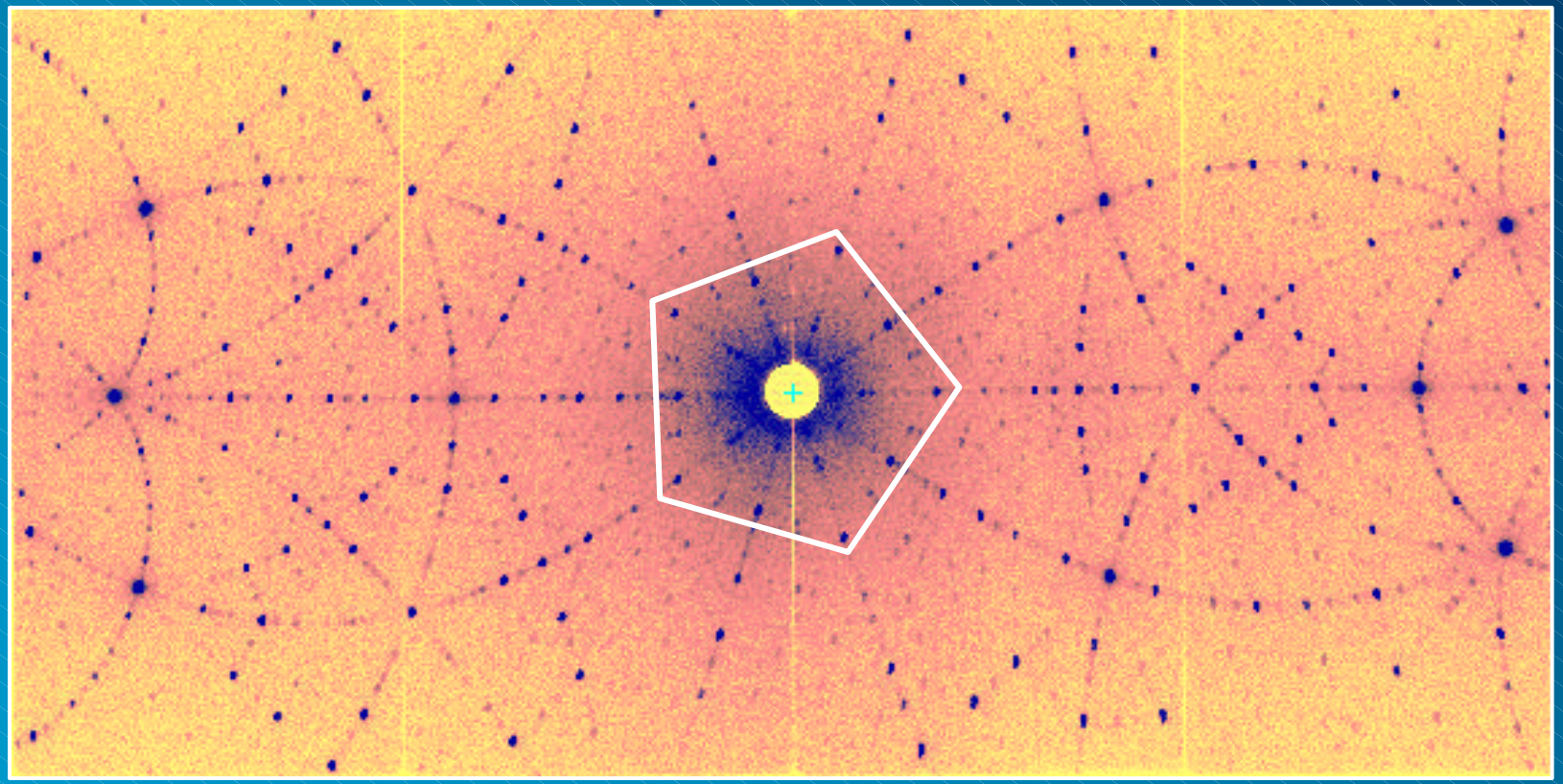
White Beam Neutron Diffraction from a single crystal

Multiple reflections sorted by the Crystal itself



VIVALDI neutron image plate photo courtesy of G. McIntyre, Oct 1999

Recipe for a High Flux Neutron Diffractometer

- A continuous neutron source
- A wide band of wavelengths
- A very high flux on the sample
- A very large area detector

ORIENT EXPRESS, a new diffractometer

Bachir Ouladdiaf, ILL Grenoble

Orient Express

On H24 thermal neutron guide

Orient Express team

- Bachir Ouladdiaf (scientist)
- John Archer (D9/D19 technician)
- Eric Bougeot-Lami (D3 technician)
- Ph. Decarpentrie (D10 technician)

ORIENT EXPRESS, a new diffractometer

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Orient Express & Bachir Ouladdiaf

On H24 thermal neutron guide

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- Bachir Ouladdiaf (D10 scientist)
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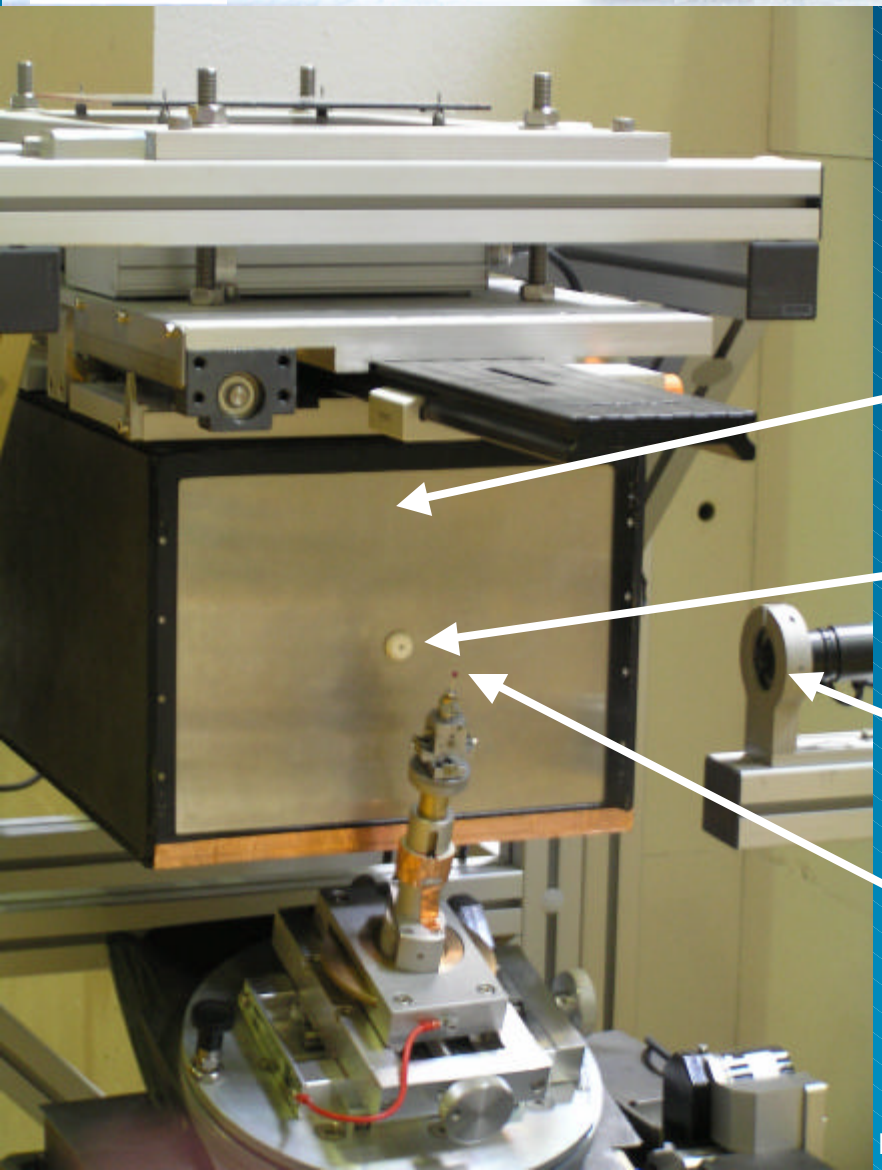
ORIENT EXPRESS, a new diffractometer

Bachir Ouladdiaf, ILL Grenoble



Orient Express

On H24 thermal neutron guide

CCD detector in backscattering

Neutron beam

TV camera for crystal alignment

Crystal on goniometer

ORIENT EXPRESS, a new diffractometer

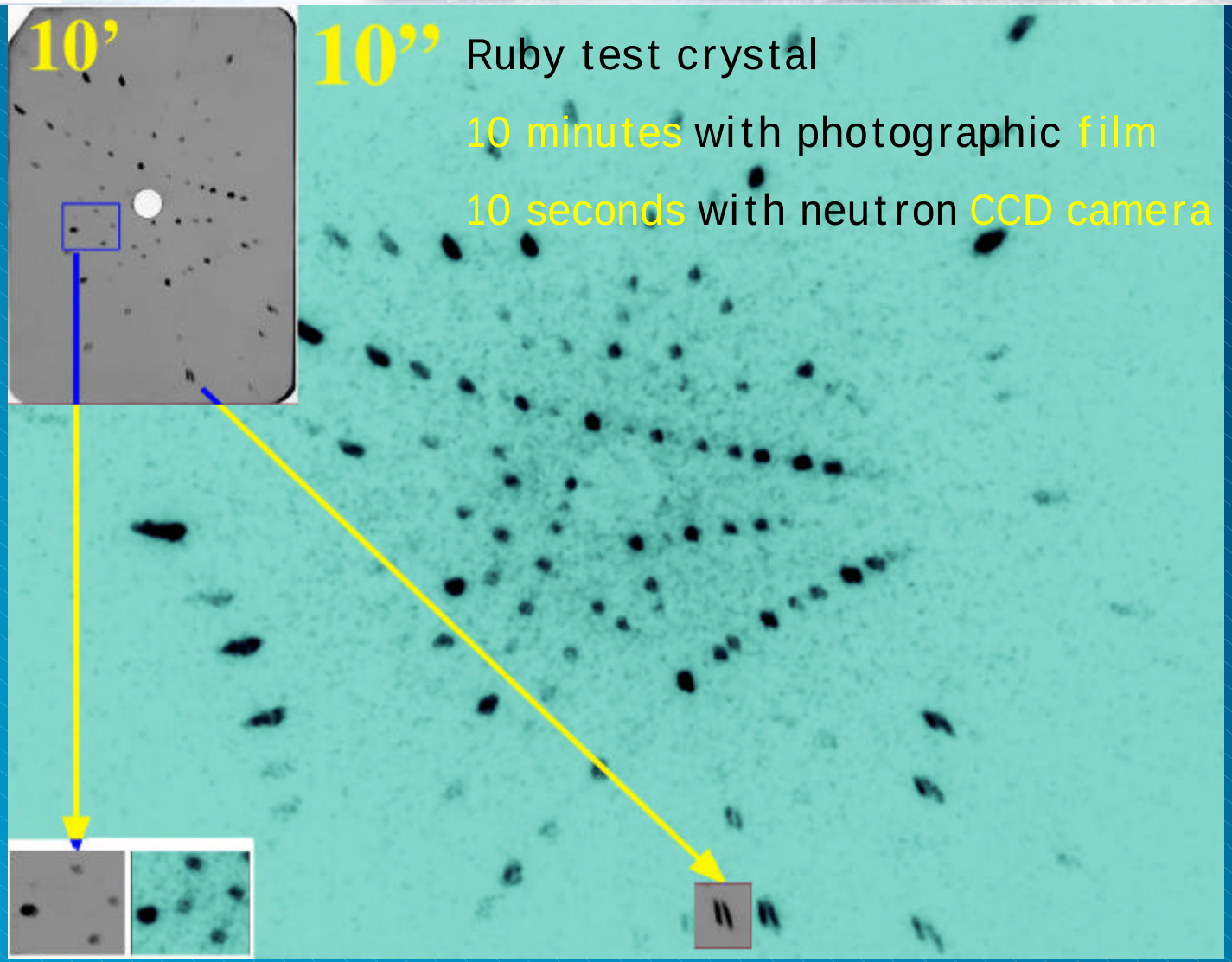
Bachir Ouladdiaf, ILL Grenoble

Orient Express & John Archer

- Simple uncooled CCD detectors
- A pair of TV cameras + computer
- Backscattering for high resolution
- Hot-cold air blower possible
- “Arndt Camera” proposed 30 years ago (cf Arndt & Willis)

ORIENT EXPRESS, a new diffractometer

Bachir Ouladdiaf, ILL Grenoble

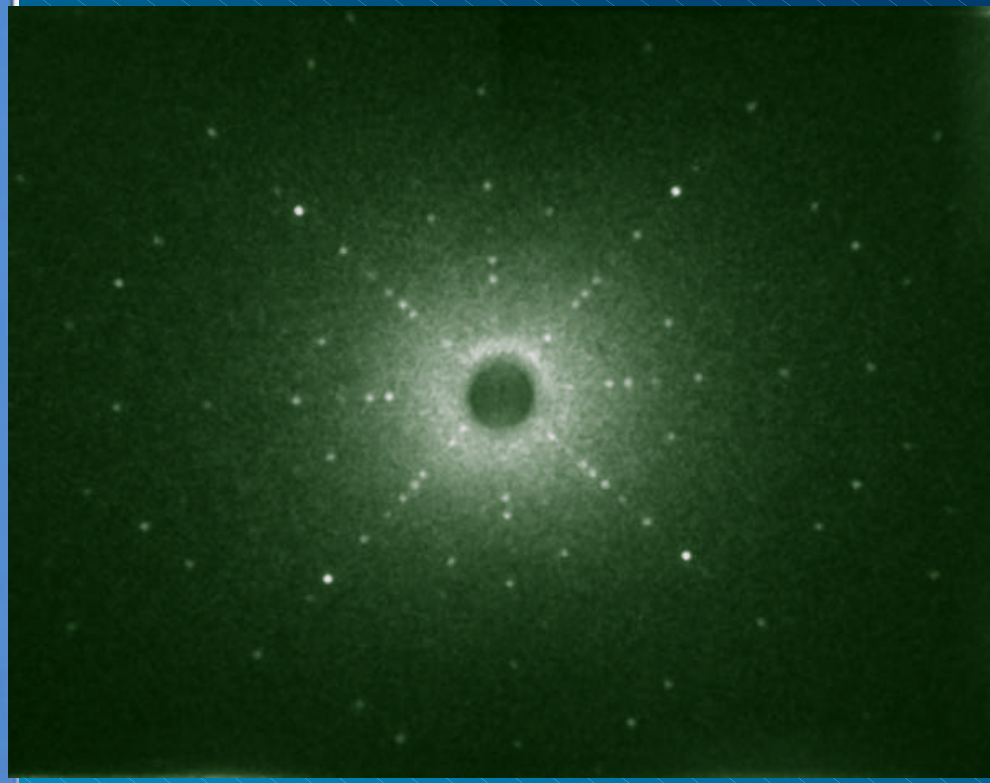


ORIENT EXPRESS, a new diffractometer

Bachir Ouladdiaf, ILL Grenoble

$GdCuO_4$ (strong neutron absorber)

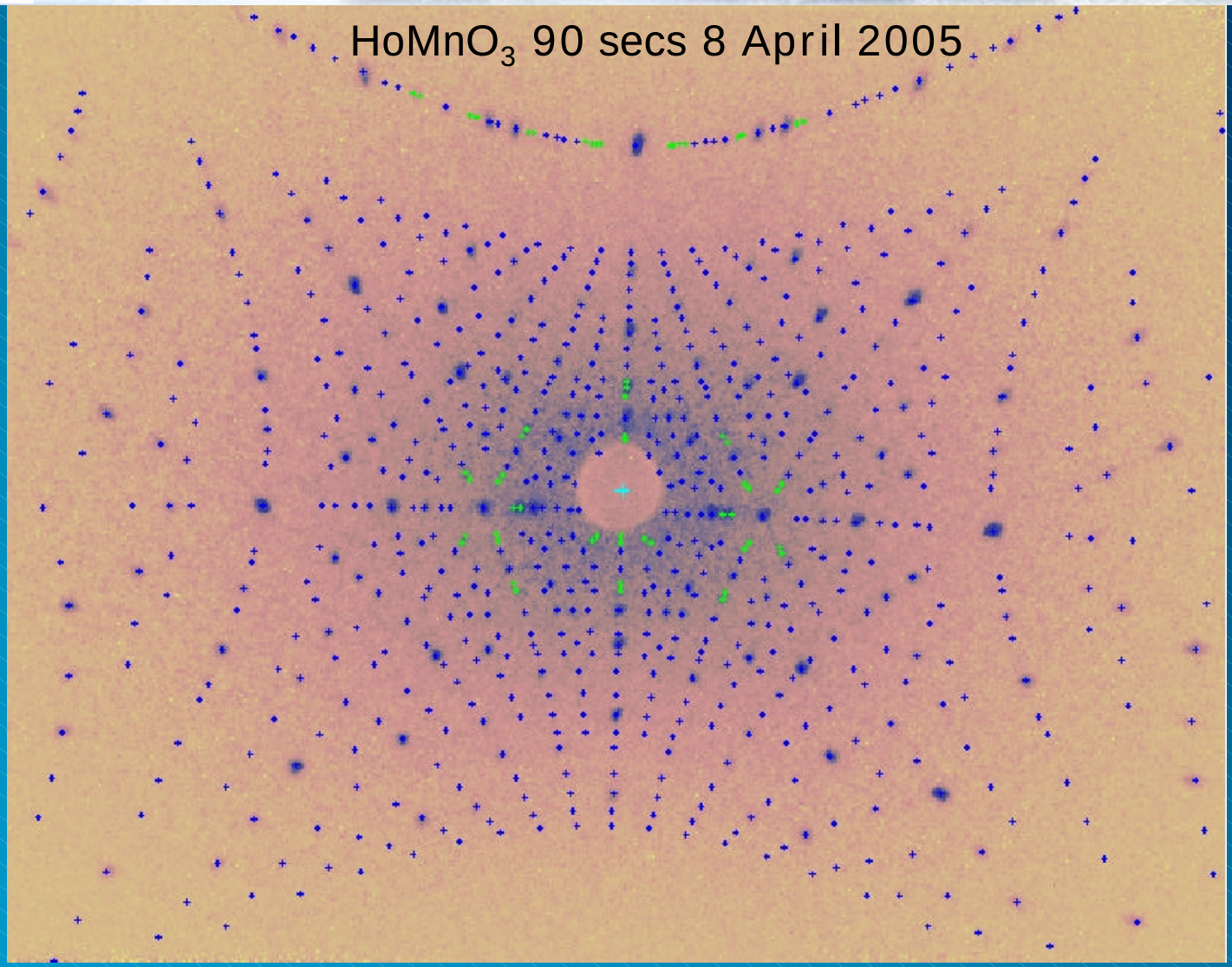
80 minutes with photographic film

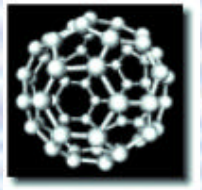


90 seconds with neutron CCD camera

$HoMnO_3$ - 90 secs on ORIENT EXPRESS

Bachir Ouladdiaf, ILL Grenoble





ORIENT EXPRESS, a new diffractometer

Bachir Ouladdiaf, ILL Grenoble

How do neutron CCD detectors compare ?

- x3 more efficient than neutron Image Plates (VIVALDI)
- Otherwise similar advantages & disadvantages
- Need cooled CCDs for low BG (we use cheap video types)
- ORIENT EXPRESS is fast and user friendly

VIVALDI, Neutron Image Plate machine

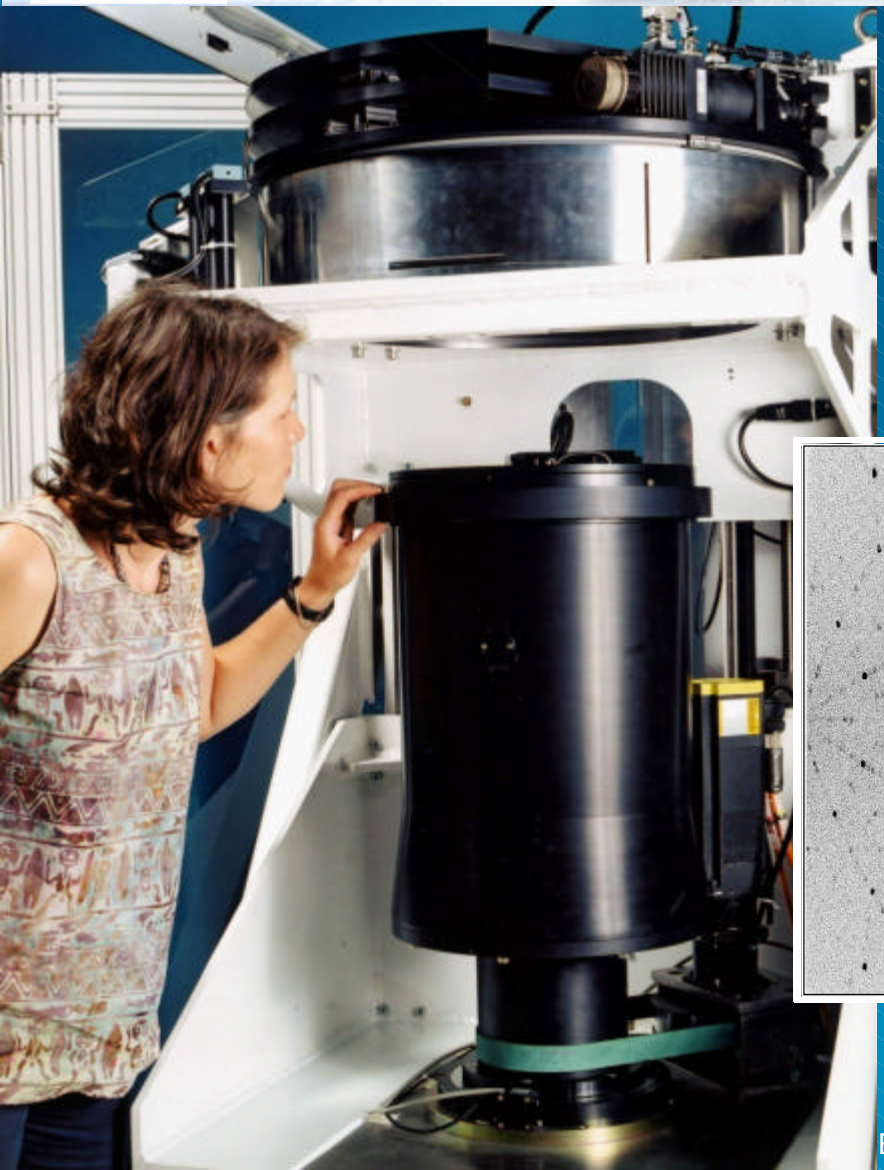
Garry McIntyre, Clive Wilkinson, ILL Grenoble

New thermal VIVALDI (2002)
On H22 super-mirror guide

"As Powerful as Powders"
G. McIntyre

VIVALDI, Neutron Image Plate machine

Garry McIntyre, Clive Wilkinson, ILL Grenoble



New thermal VIVALDI (2002)
On H22 super-mirror guide

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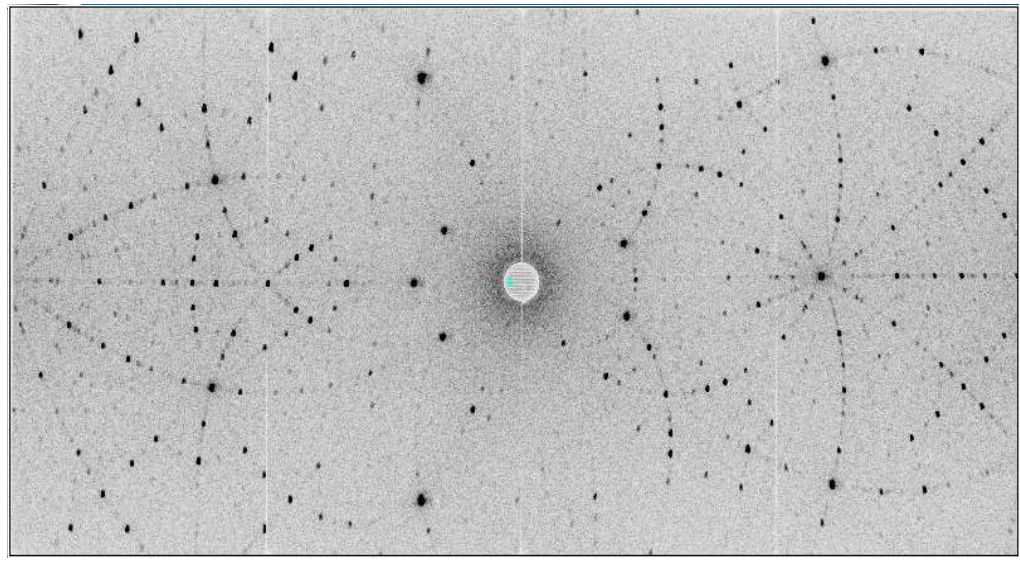
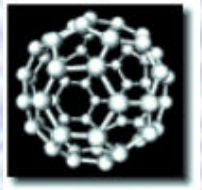




VIVALDI, Neutron Image Plate machine

Garry McIntyre, Clive Wilkinson, ILL Grenoble

First experiments on VIVALDI

Very fast data collection over all of reciprocal space for very small samples

Compound	Volume (mm^3)	Unitcell ($Å^3$)	Expose (hr)	No. Peaks	I / s (I)	Total (hr)
Vitamin B12	6	8853	2	7596	10.1	60
$Cs_3VCl_6.4H_2O$	2	446	0.7	647	6.6	3
$Na_2Pb(OH)_2$	2	147	0.8	263	7.9	5
$LiAlSi_2O_6$	1.4	389	0.33	442	11.9	2
$Co(NH_3)_6.CuCl_5$	1	2691	0.7	1865	6.0	3
$Co_4C_{22}H_{36}$	0.6	8254	2.5	4340	4.8	22
$dabcoHBF_4$	0.21	473	1	384	5.0	10
$Cd_2Nb_2O_7$	0.07	279	2	204	3.1	*
$C_4H_4N_2O_2$	0.00075	451	4	272	1.1	48
$(NH_4)_2Cr(SO_4)_2.6H_2O$	3.5**	726	1	557	5.6	4

**10 kbar TiZr pressure cell !!

SALSA, Neutron Strain Scanner

Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)

SALSA – It's Hot

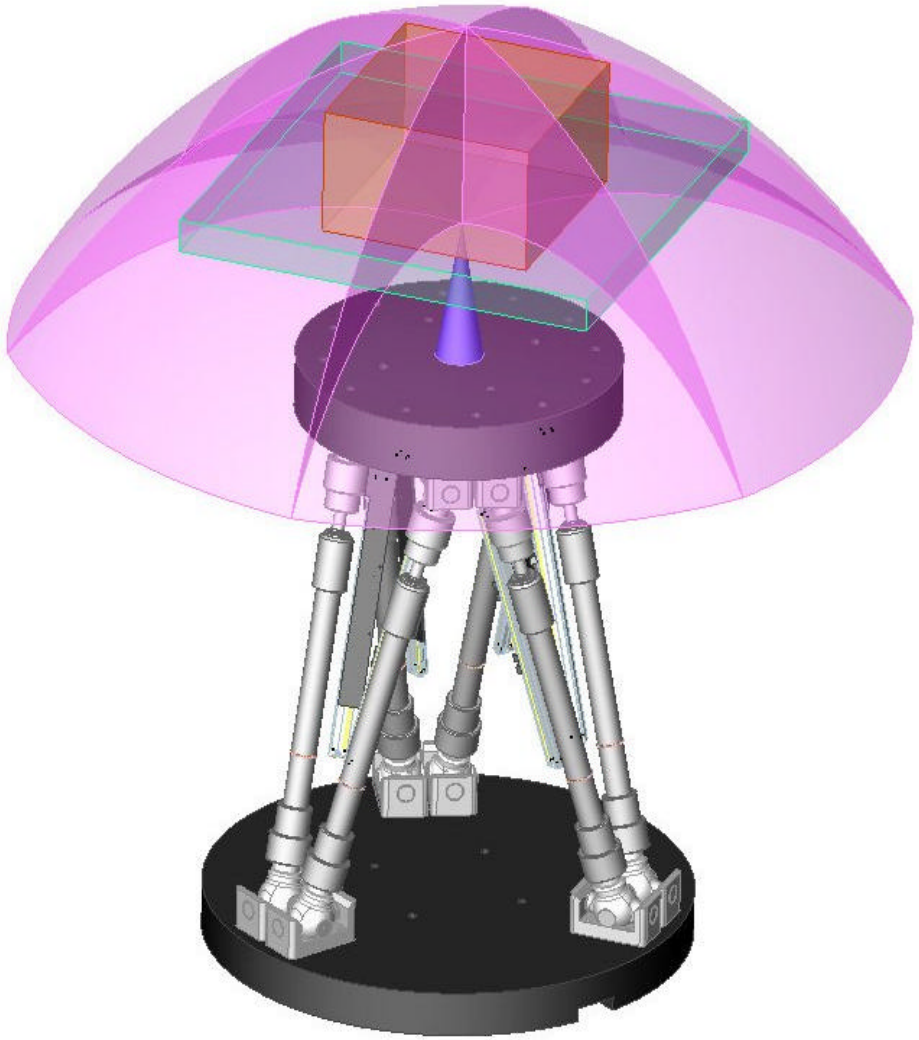
On H22 super-mirror thermal guide

The all-singing & dancing Strain Scanner

- High neutron flux
- Samples up to 500 kg weight.
- Stewart Platform (hexapod)
  very strong, yet very precise.

SALSA, Neutron Strain Scanner

Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)



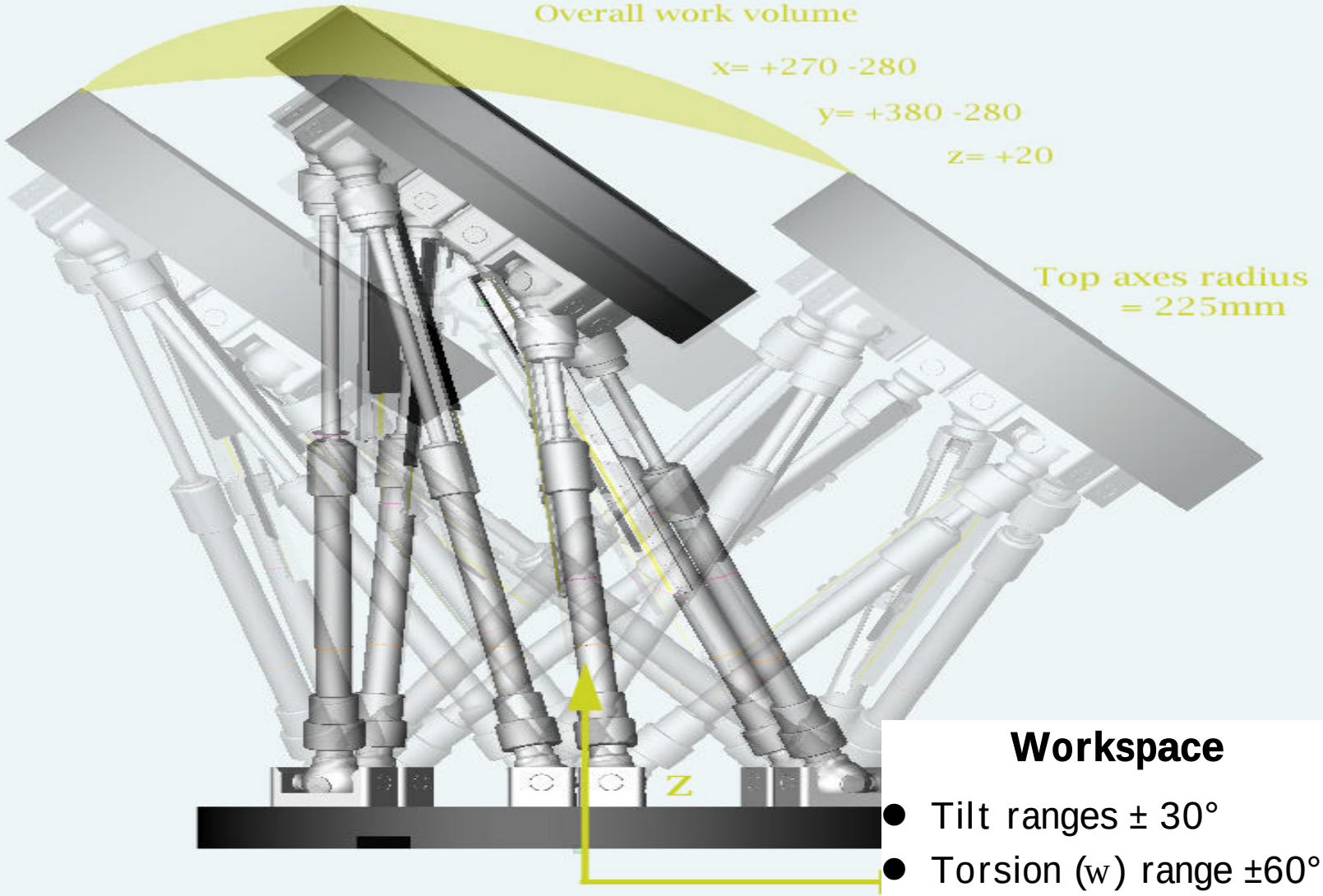
SALSA – It's Hot

On H22 super-mirror thermal guide

- Stewart platform (Hexapod)
- High flexibility
- Laser/Camera system
- Max. load 500 kg
- Air pads

SALSA, Neutron Strain Scanner

Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)

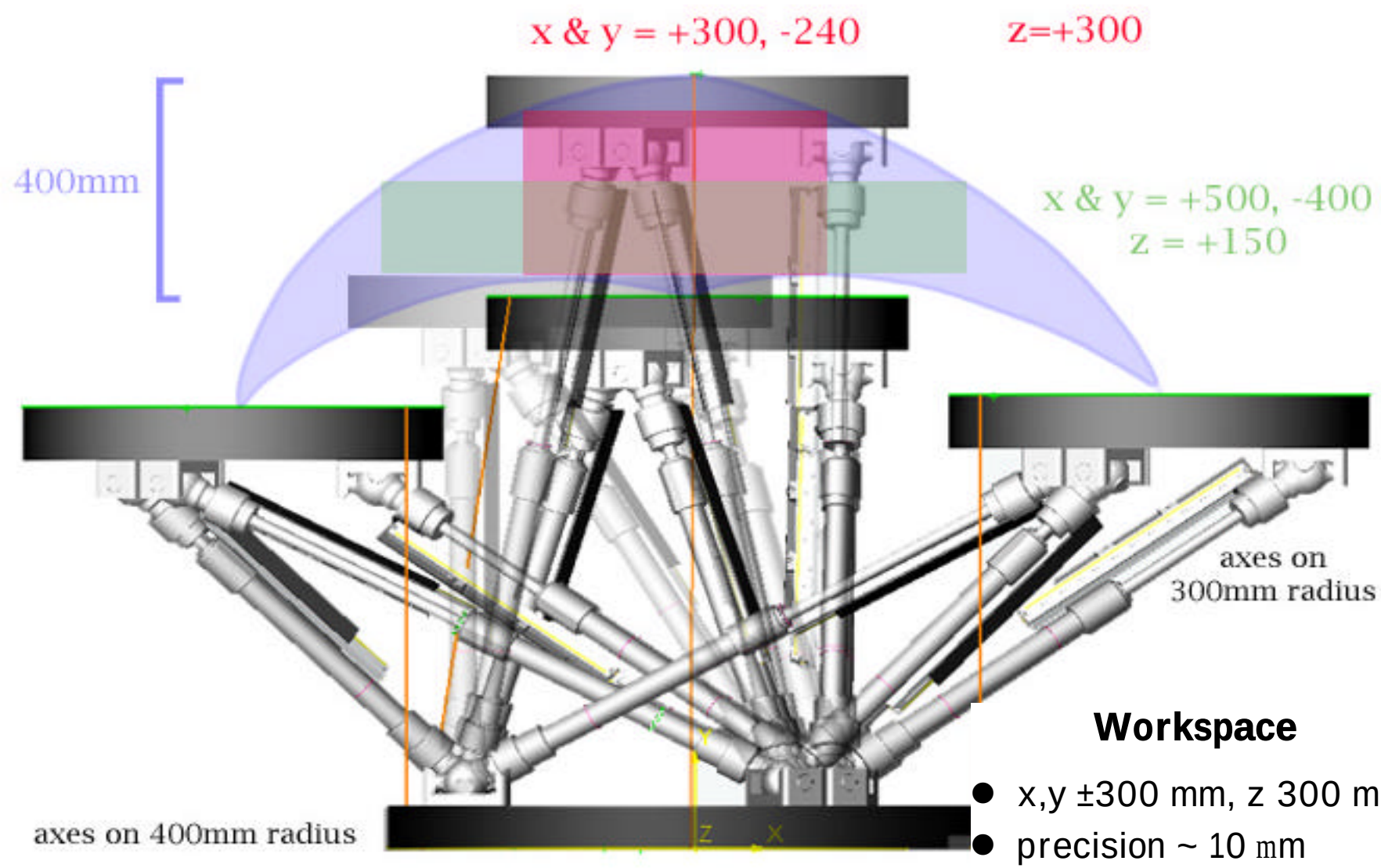


Workspace

- Tilt ranges ± 30°
- Torsion (w) range ±60°

SALSA, Neutron Strain Scanner

Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)



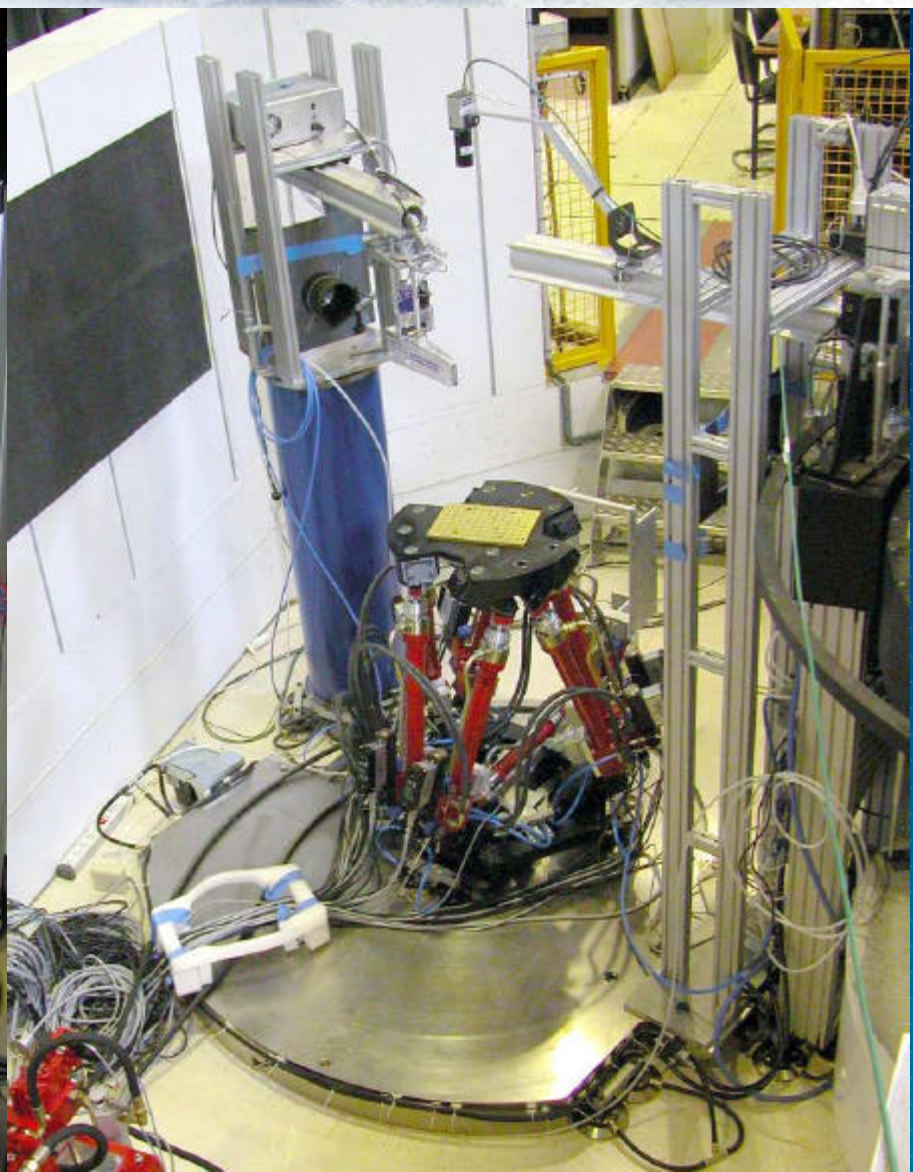
Workspace

- x,y ±300 mm, z 300 mm
- precision ~ 10 mm

SALSA, Neutron Strain Scanner

Ph. Withers, G. Bruno (Manchester), Th. Pirling (ILL)

Mark Jacques &
SALSA Hexapod



SALSA, Neutron Strain Scanner

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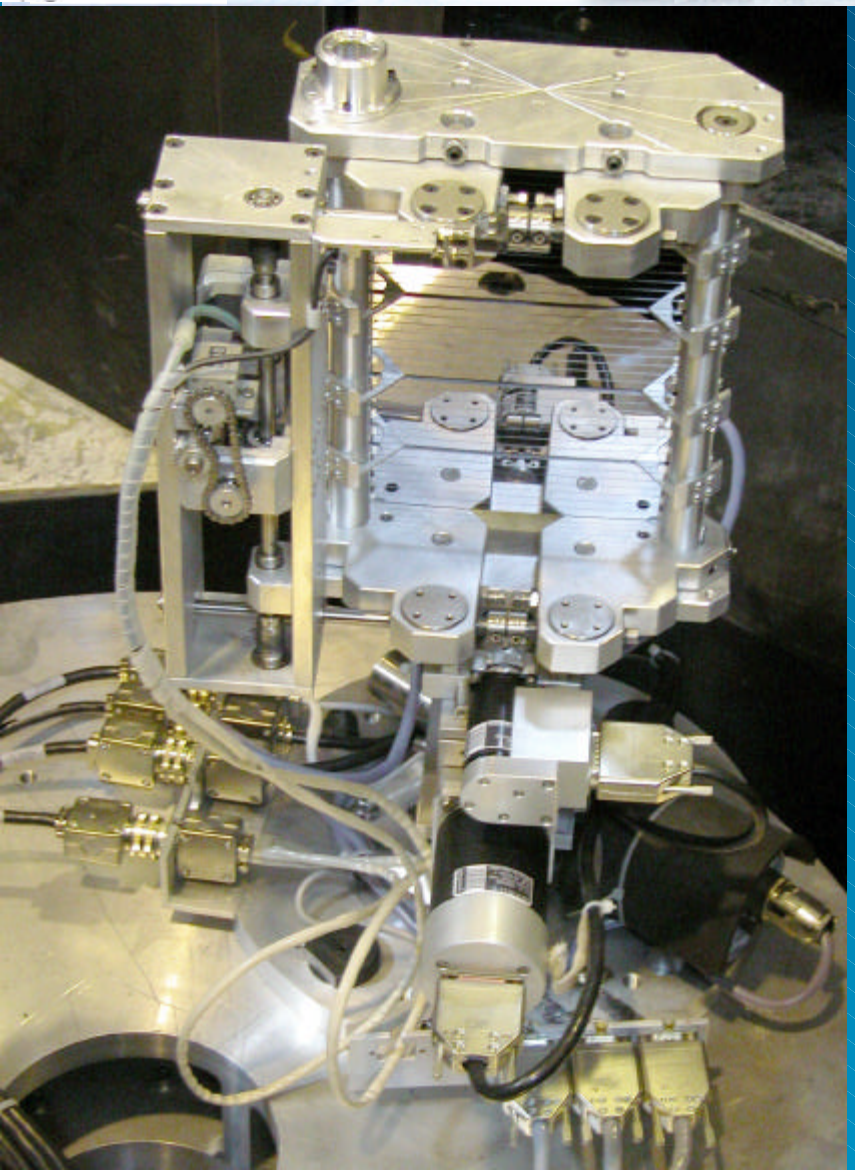
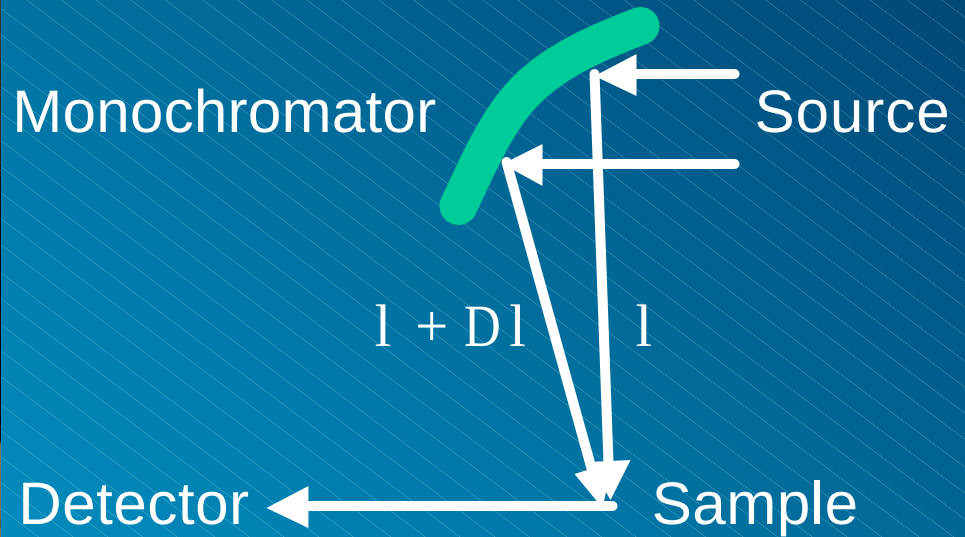


Double-focusing bent perfect Si-monochromator

On H22 super-mirror thermal guide

- Very large Dl/l, high flux on sample



SALSA, Neutron Strain Scanner

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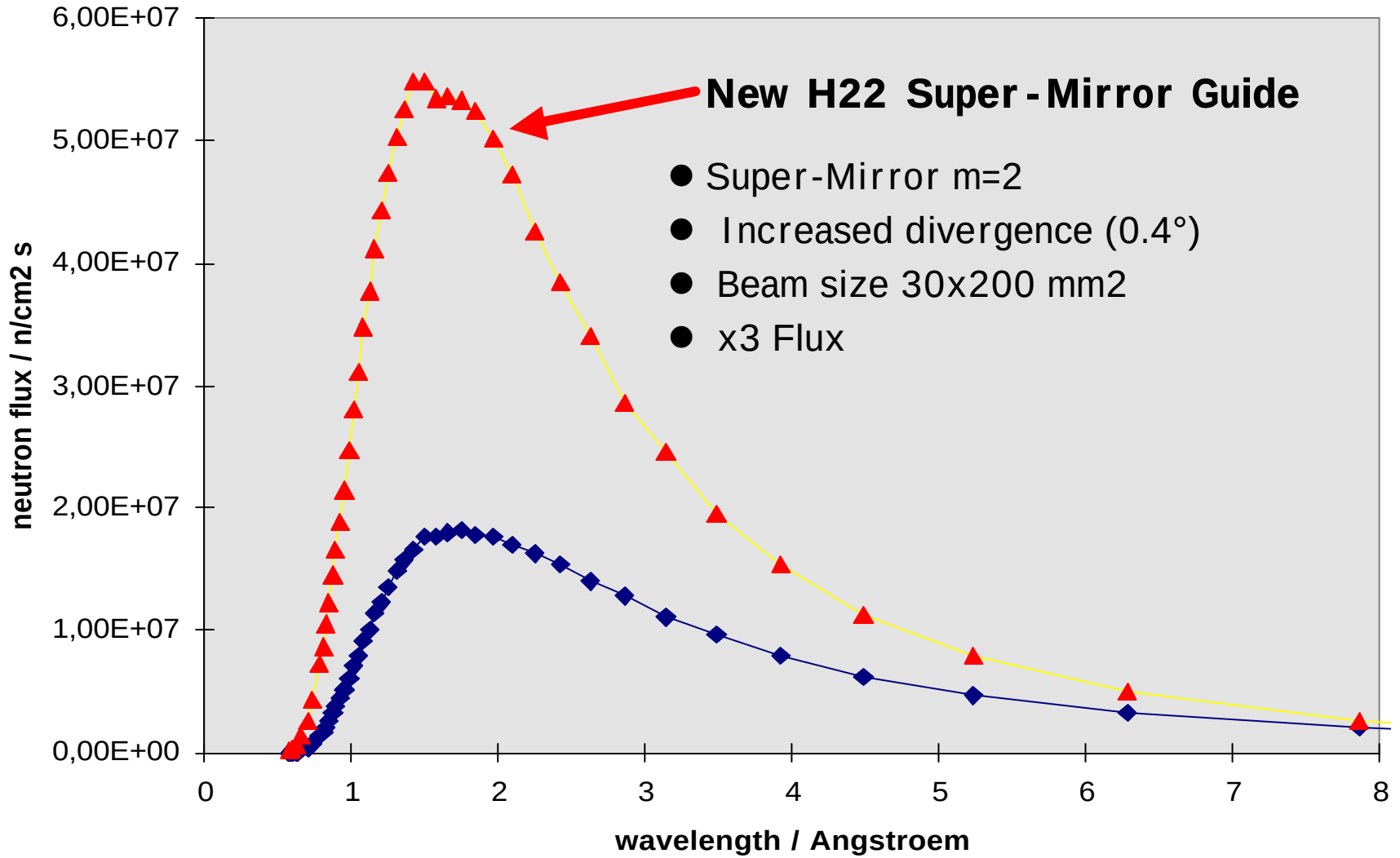

High Flux Neutron Diffractometers

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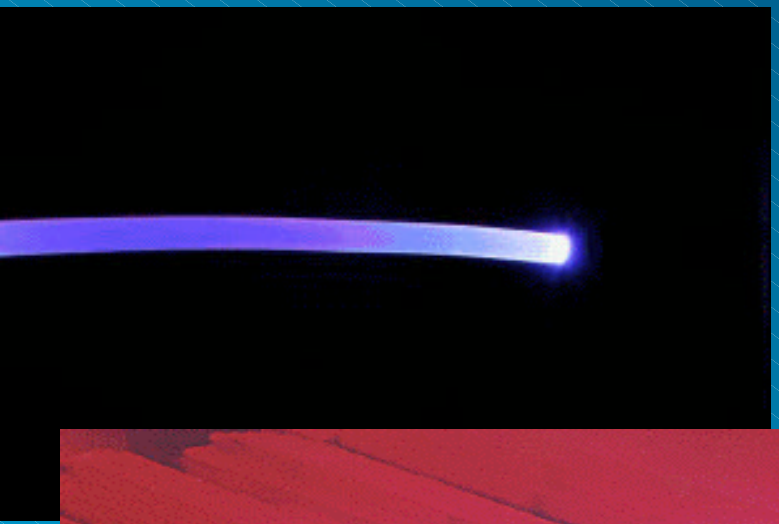
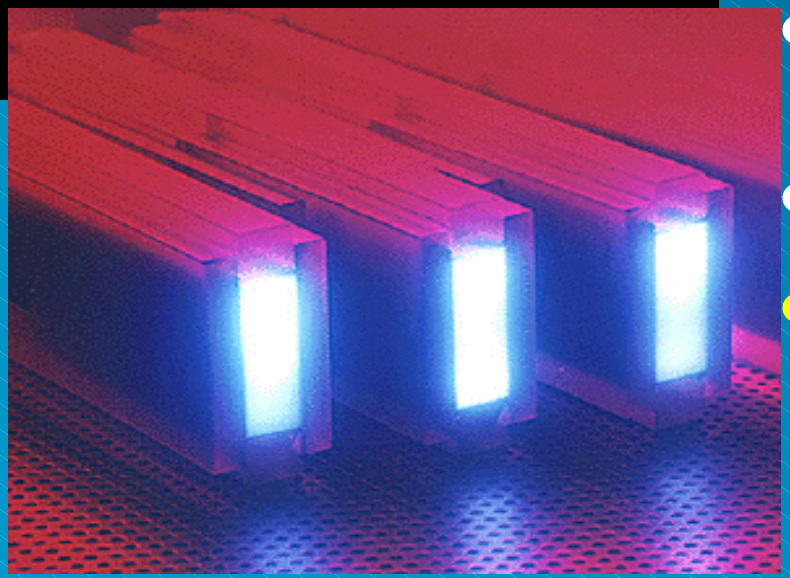
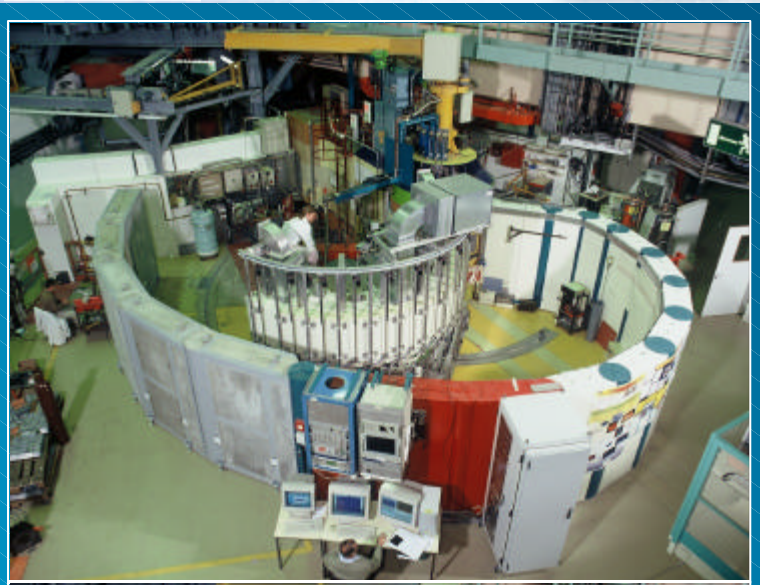
New H22 Super-Mirror Guide for D1A, D1B, SALSA, VIVALDI

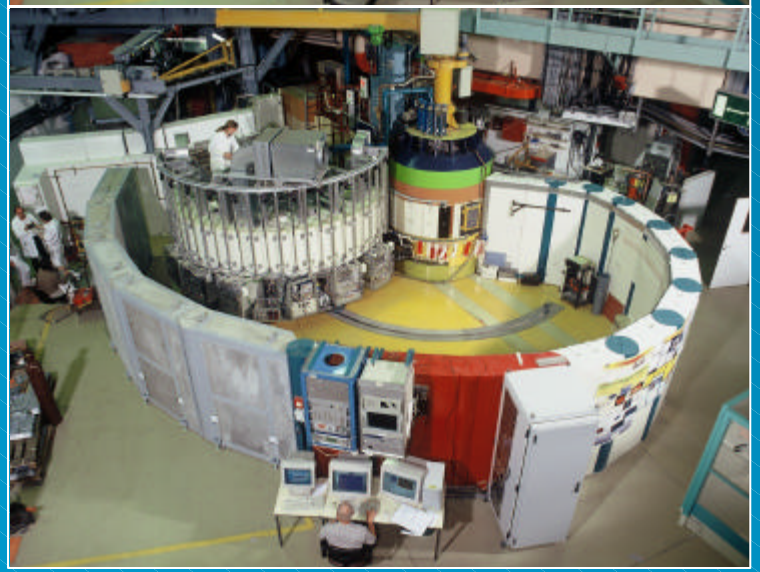


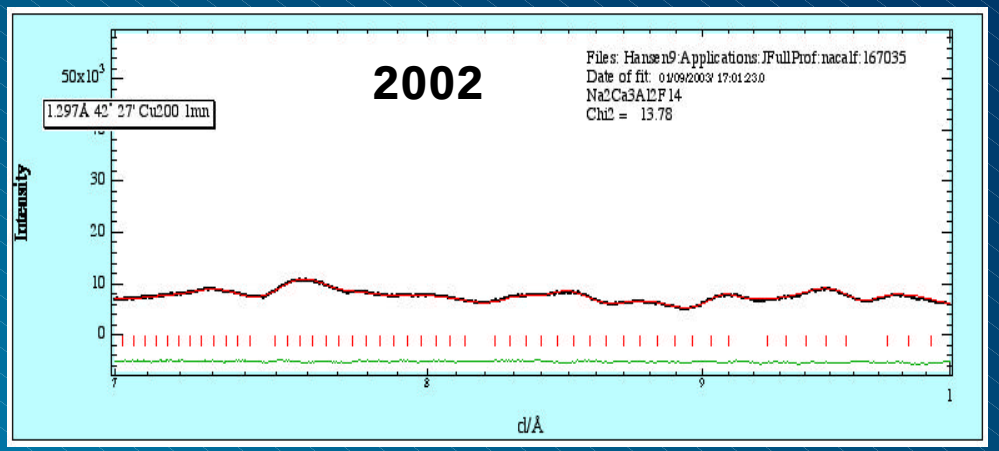


- Neutron guide tubes bring the neutrons to the experiment
  cf optic fibres
- Super-Mirrors increase the solid angle
  cf multiple optical coatings on lenses
- New H22 super-mirror guide (2005)
  x4 flux for D1A,D1B,SALSA,VIVALDI
- Already half finished, complete 2005
- However, there is a new proposal to replace all thermal guides by a 3rd ILL cold source.

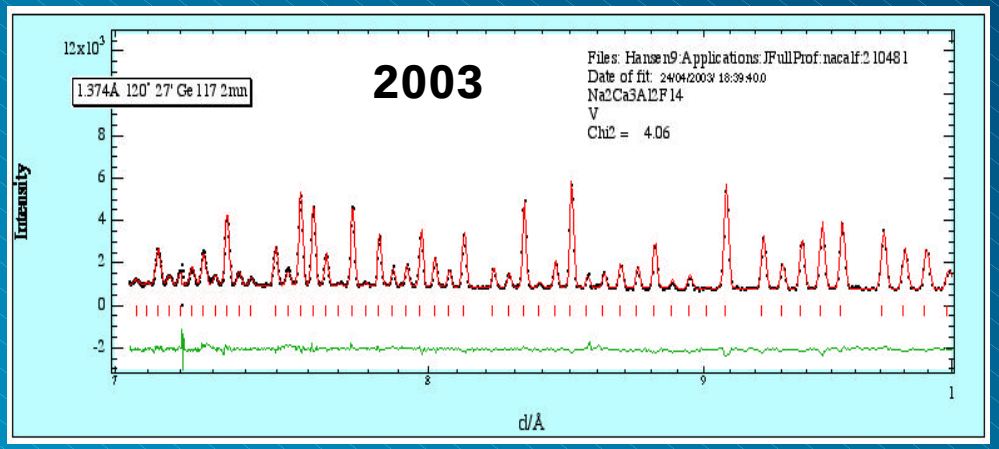
High flux compatible with good Resolution
High take-off option on D20







Before and After (data in 2 min.)



Higher D20 resolution since 2003

Applications - fast detectors, small samples

Very fast chemical and electrochemical kinetics

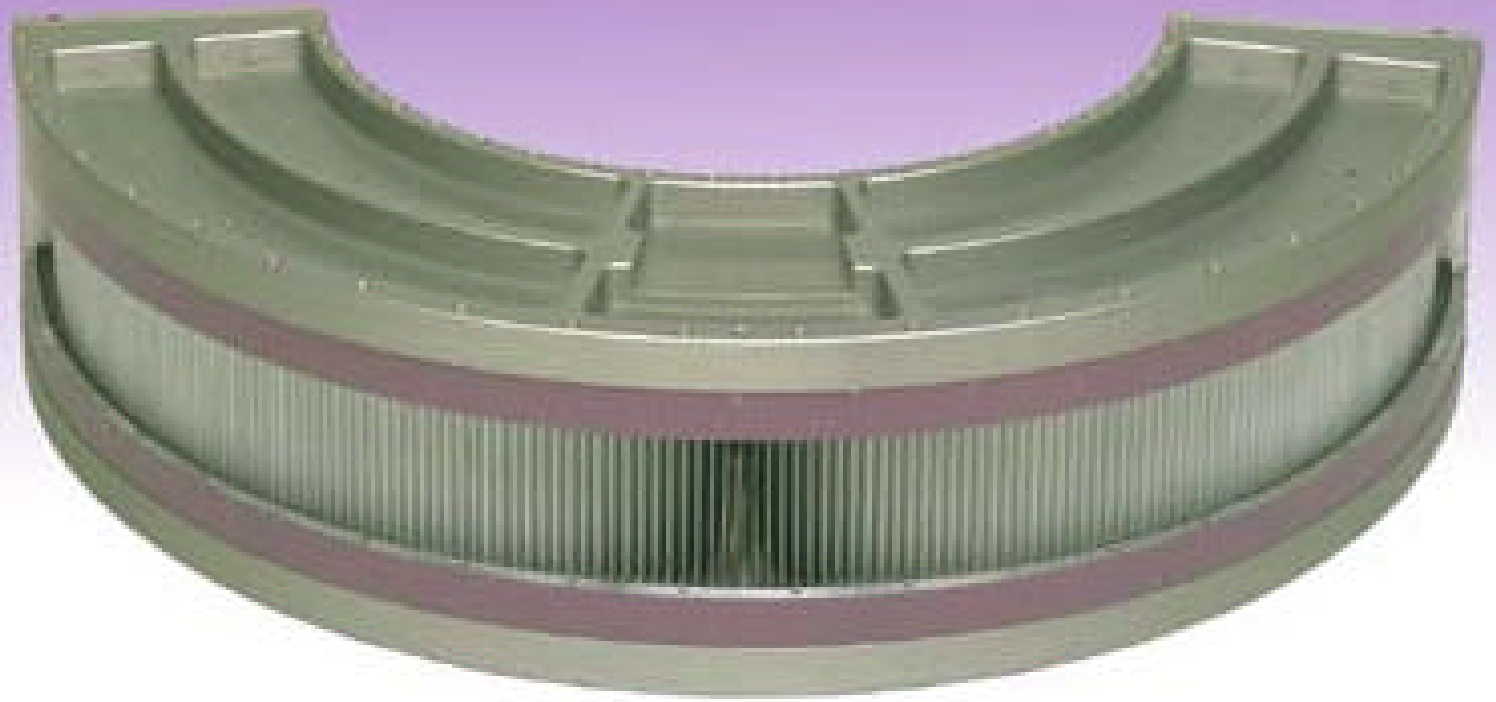
- The explosive SHS reaction was studied in real time with neutrons
- The reaction is exothermic, & heats the sample to 2200°C in <1 sec
- The complete diffraction pattern (left) is collected at 300 ms intervals - **A World Record**

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

New radial collimator for D20
New high pressure cell

cf radial collimators on ISIS-GEM, PSI-HRPT etc

New Paris-Edinburgh pressure cell



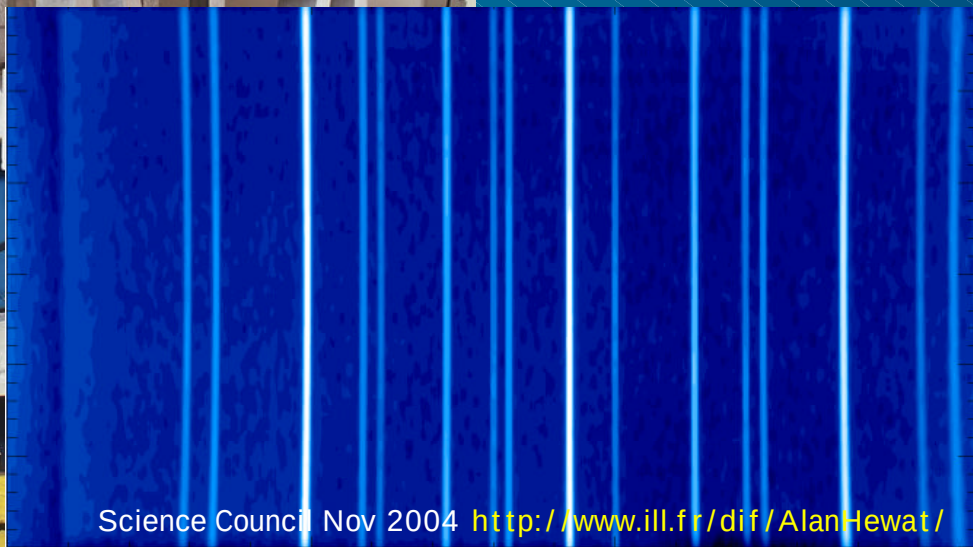
Super-D2B Millennium Project
High resolution 2D-detector

New D2B-2003
Very High Res.
X6 intensity

1st 2D detector

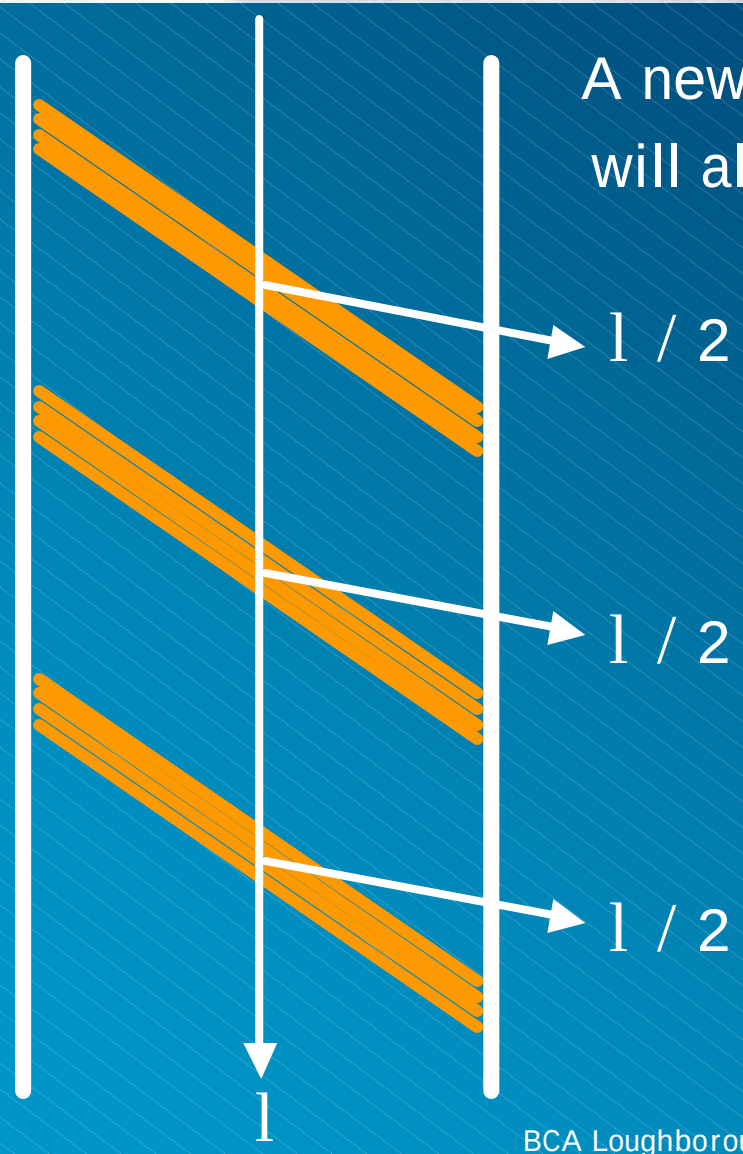
For Neutron PD

Integrate over Diffraction Cones



Science Council Nov 2004 http://www.ill.fr/dif/AlanHewat/

Super-D2B Millennium Project – Part II
Larger choice of wavelengths & d-spacings



A new type of graphite filter will allow λ=6.0Å, 3.0Å, 2.4Å

D19 Millennium Project
Large 2D detector for biological structures

New D19 - 2004

The Future for ILL

DRACULA, D9, D16

D19 Millennium Project
Large 2D detector for biological structures

Complete D19 detector, 11 April 2005

ILL Diffraction Needs a 2nd Thermal Beam

Diffractometer for

Rapid

ACquisition over

Ultra

Large

Areas

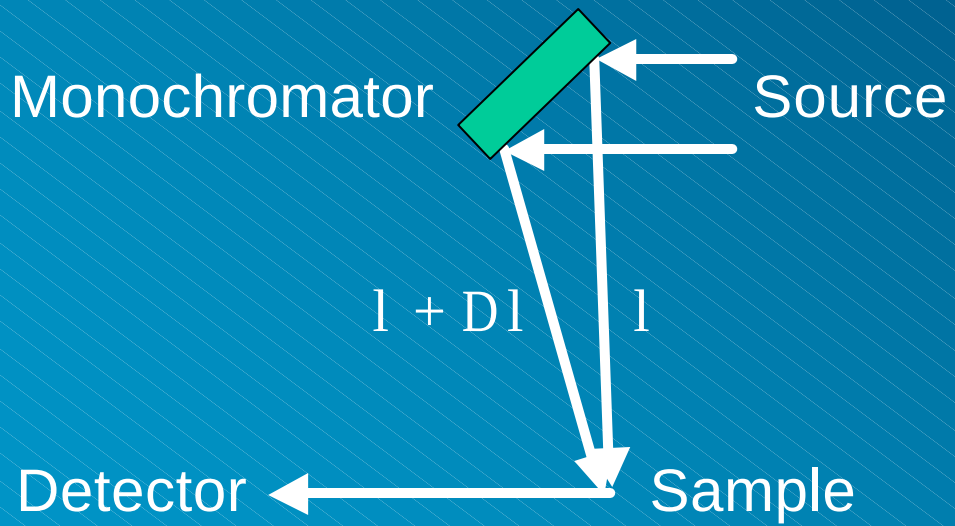
DRAC, first presented at the ILL "Instrument Day" 26 Feb 2002

DRAC, highest priority for Instrument Committee 17 Oct 2003

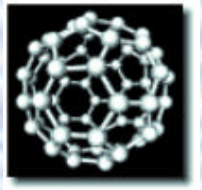
Why is sample flux so high from a reactor?

Large wavelength-band focusing monochromators

Focusing in reciprocal space can give a factor of x10



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



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.

	D20	GEM	DRACULA	SNS
Flux average on sample	$5x10^7$	$\sim 2x10^6$	$\sim 10^8$	$\sim 2.5x10^7$
Detector solid angle	0.27 sr	4.0 sr	1.5 sr*	3.0 sr
Efficiency=Flux*Detector	1.7	1	18	9

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

High Flux Neutron Diffractometers

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Register now on: http://www.ill.fr/dif/epsrc/

Spring 2005 Conference on EPSRC-ILL Millennium Projects

May 25-27 at ILL Grenoble France