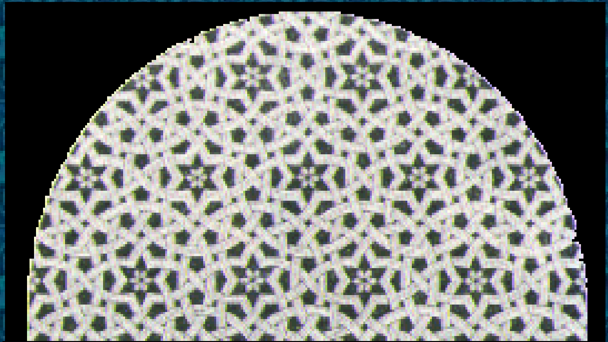
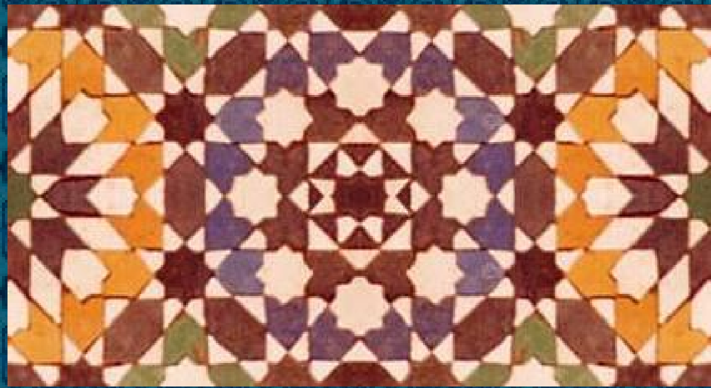
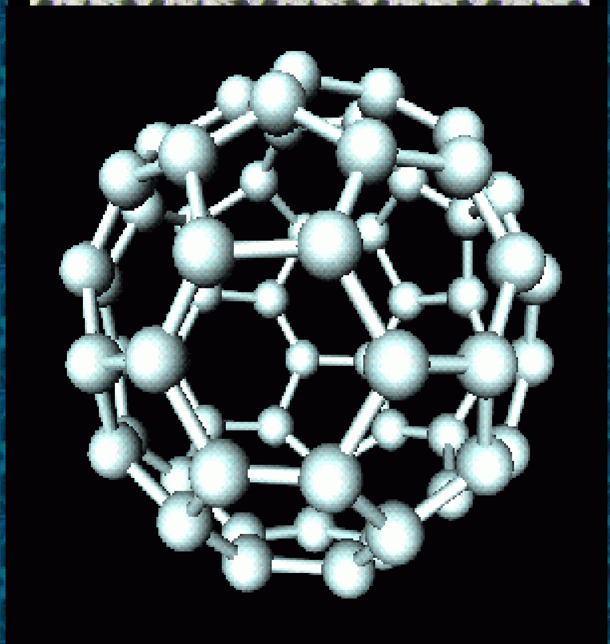
Mathematics, geometry, symmetry & the structure of materials

Arabesque

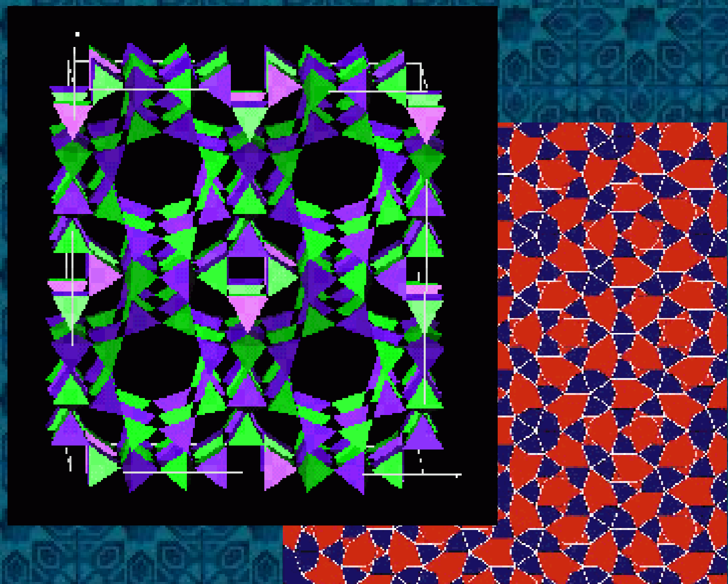


Moroccan star tiling





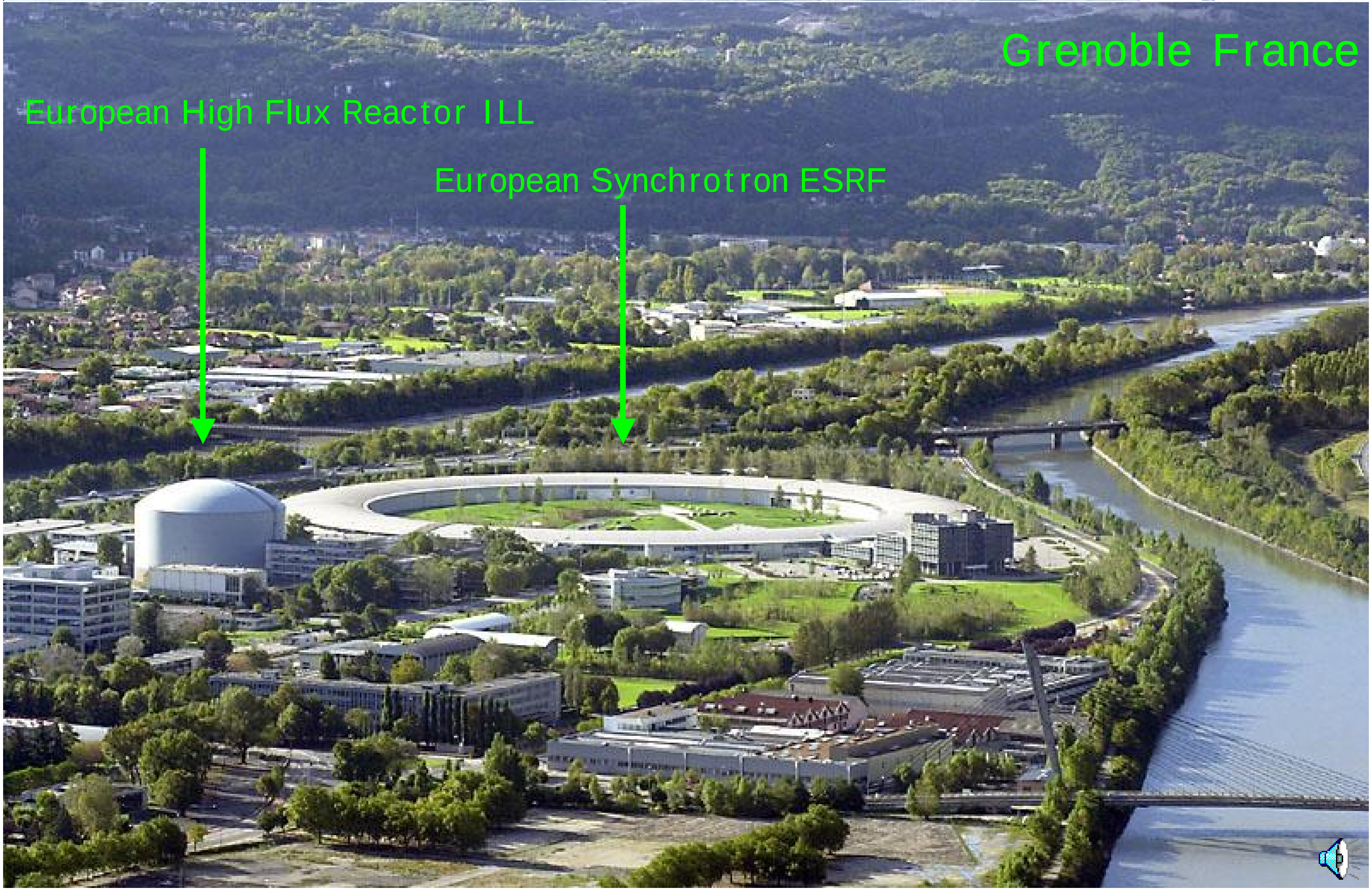
Carbon-60



Crystals & Quasicrystals

- World's most intense neutron source
- 1280 visiting scientists each year
- 300+ scientific papers each year
- physics, chemistry, biology, materials

ILL member countries are shown in green

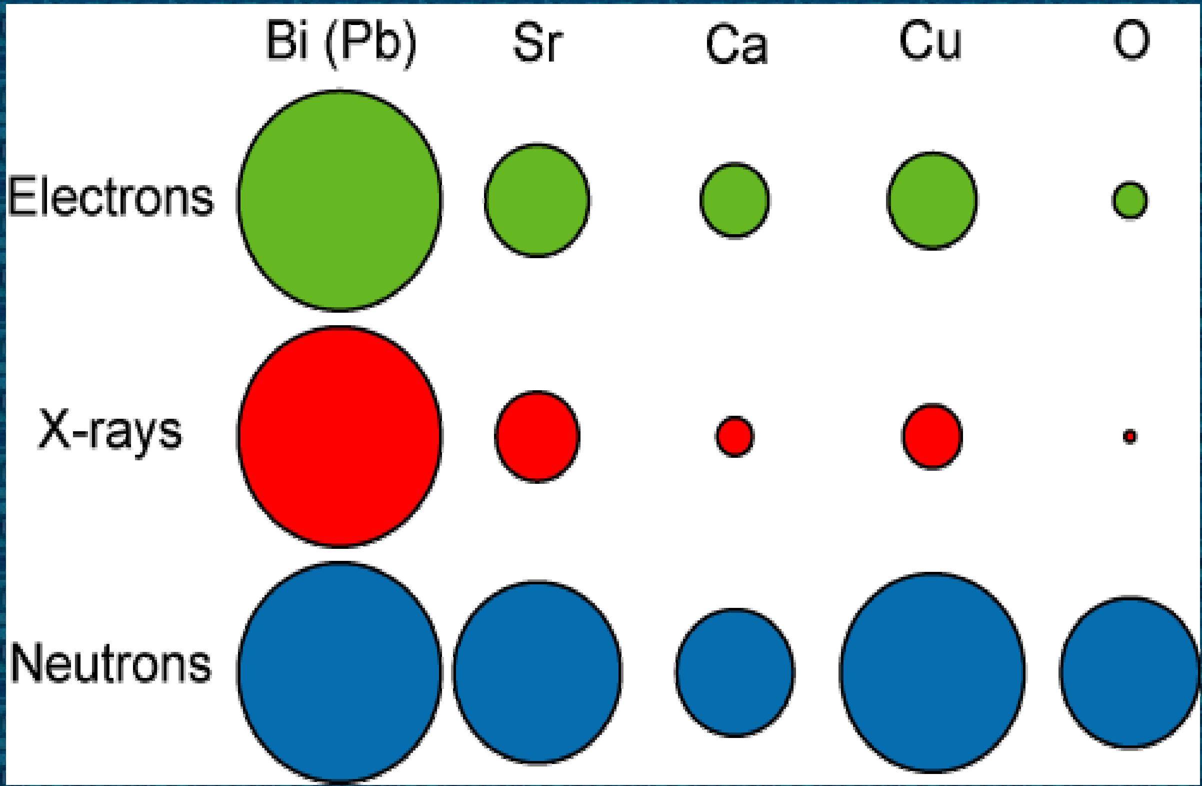

Grenoble France
European High Flux Reactor ILL
European Synchrotron ESRF

Why Neutrons ?

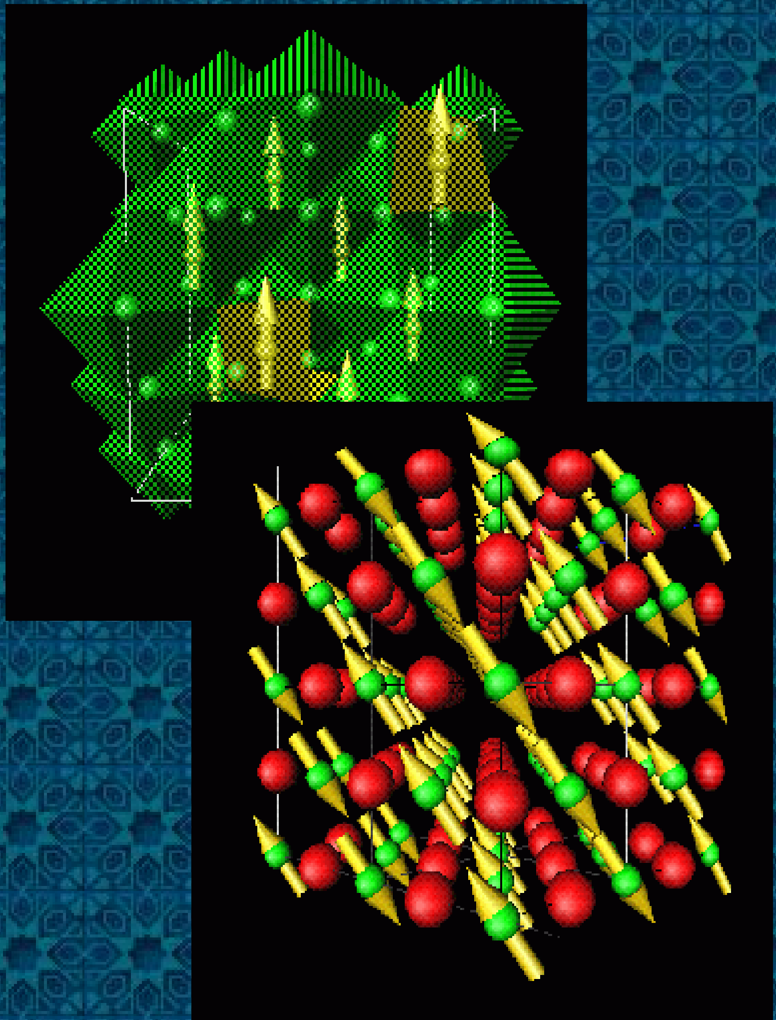
- Neutrons act like both particles and waves
- Neutrons are electrically neutral & more penetrating than X-rays.
- Neutrons interact with nuclei & locate atoms more precisely.
- Light atoms scatter neutrons as strongly as heavy atoms.
- Neutrons are tiny magnets, & can determine magnetic structures.
- Neutrons can study atom dynamics & the forces between atoms.

Neutrons scatter strongly from light atoms

- Neutron scattering is of similar magnitude for all atoms
- X-ray scattering is proportional to the number of electrons
- Electron scattering depends on the electrical potential

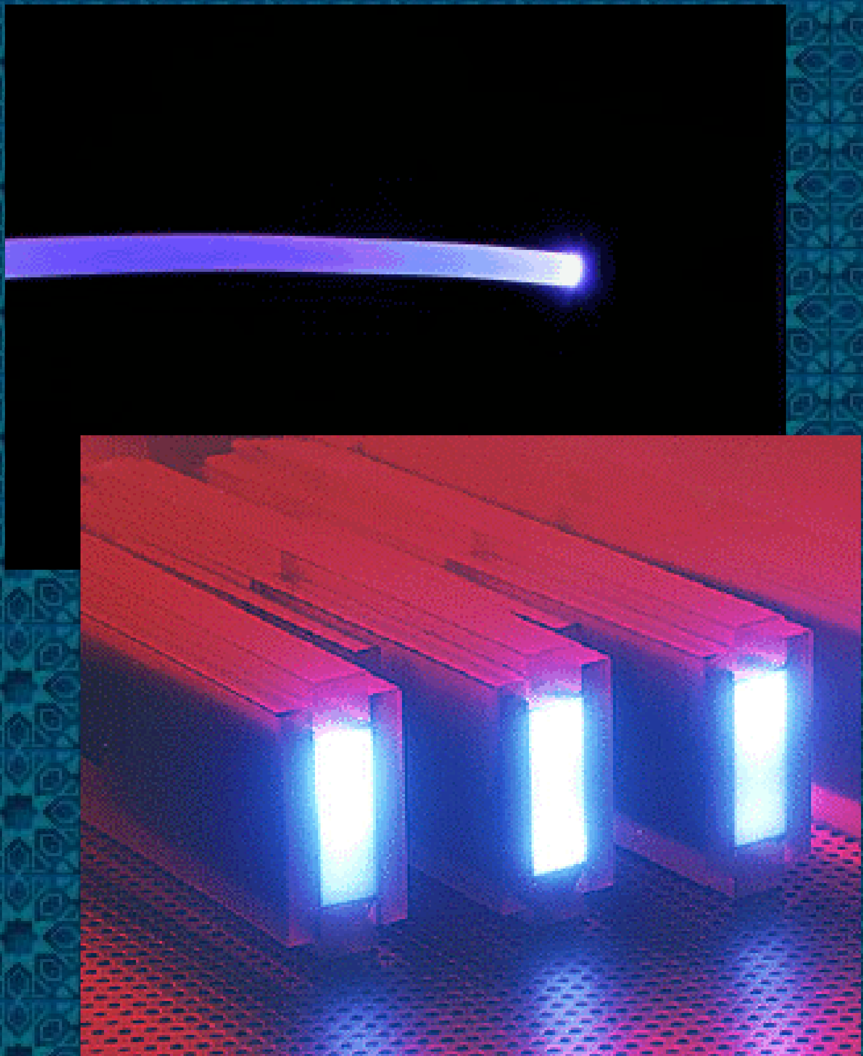


Neutrons scatter strongly from magnetic materials



- Neutrons act like tiny magnets
- Interact with atomic magnetic moments
- Neutrons determine magnetic structures
- Ferromagnetic magnetite Fe_3O_4 (top)
- Antiferromagnetic manganese oxide MnO

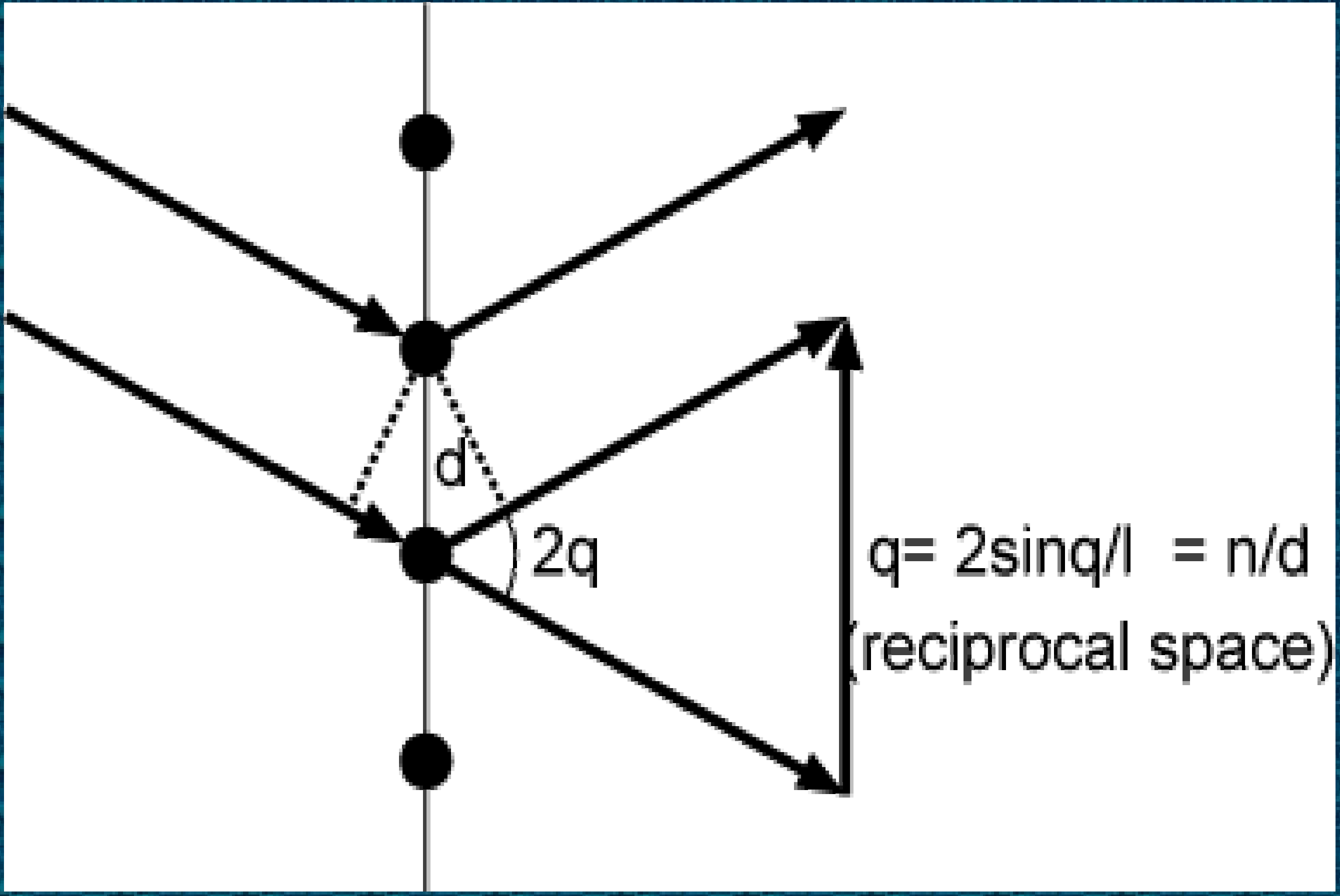
Neutrons can be transmitted like light in an optic fibre

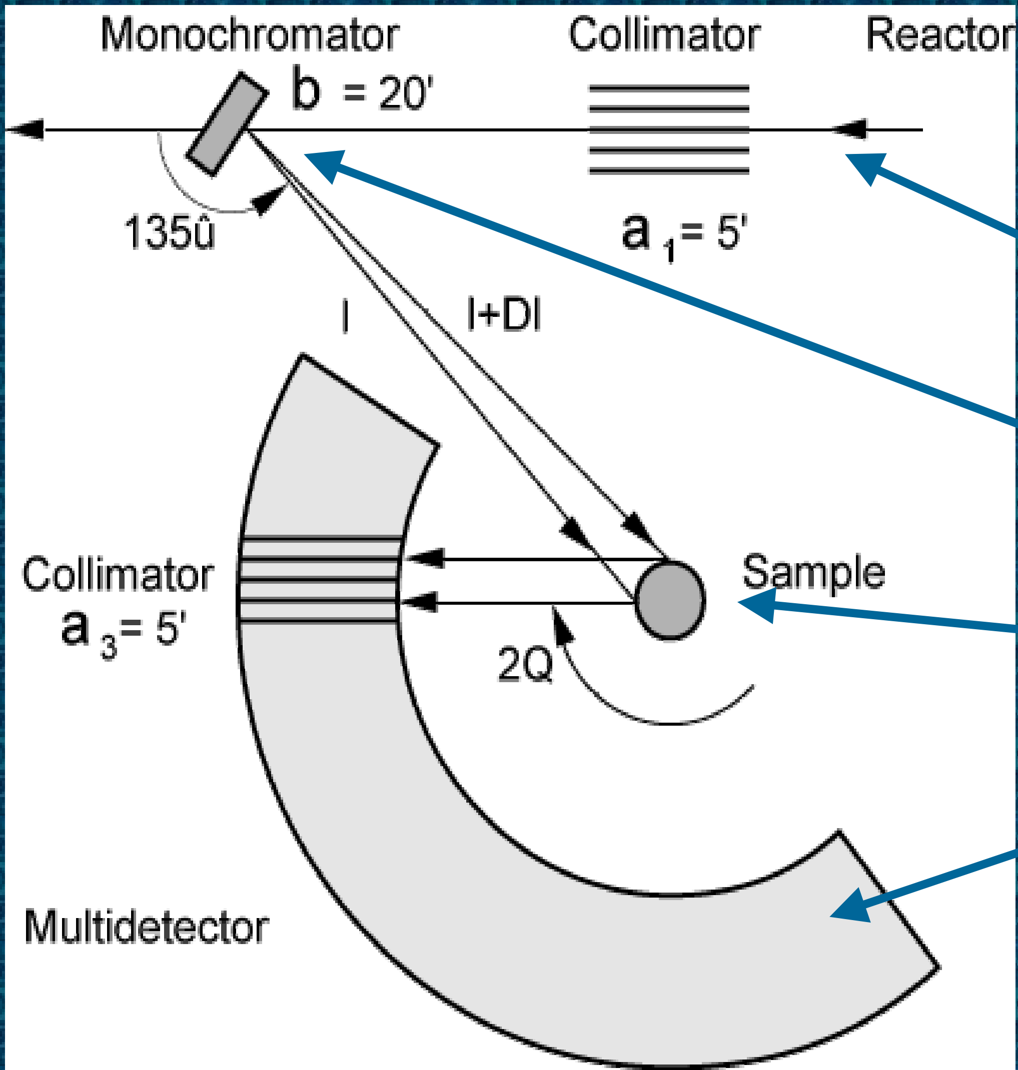


- "Neutron guide tubes" bring the neutrons to the experiment
- The transmitted intensity (solid angle) depends on the neutron wavelength
- Only neutrons are transmitted (low background).

Neutrons scatter like waves from atomic planes

- The neutron wavelength is similar to the atomic spacing
- Scattered neutrons determine the atomic structure of materials



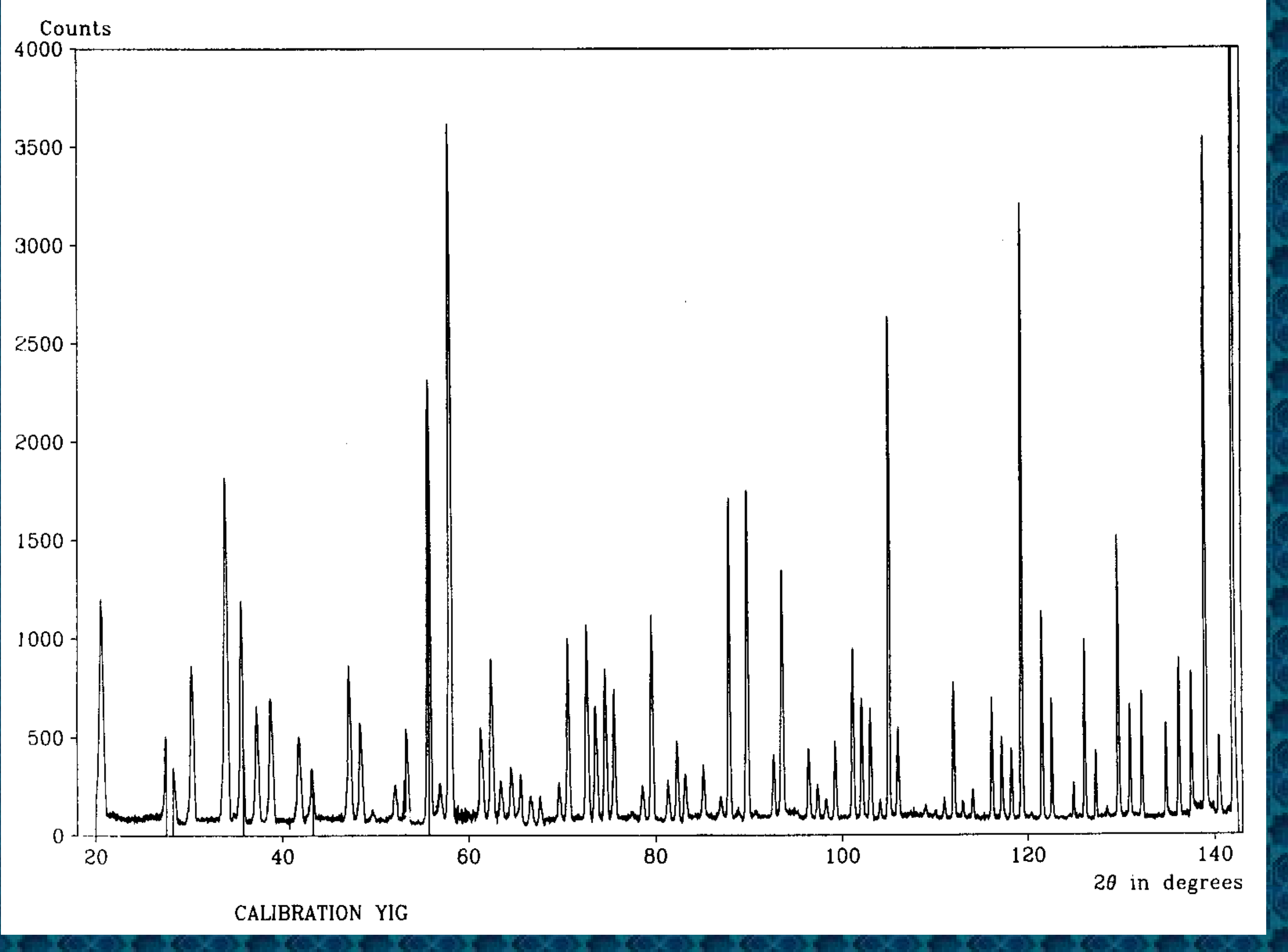


Neutron diffractometers are simple

- A "white" beam of neutrons from the reactor is collimated
- A large focussing monochromator selects particular wavelengths
- This small band of wavelengths is scattered by the sample
- A large multi-detector collects the neutrons scattered at all angles

High resolution neutron diffractometers – D2B at ILL

Strong peaks at high angles give high precision structures of materials



Neutron intensities are low, so large detectors are needed

Construction of a microstrip position-sensitive detector (printed circuit)

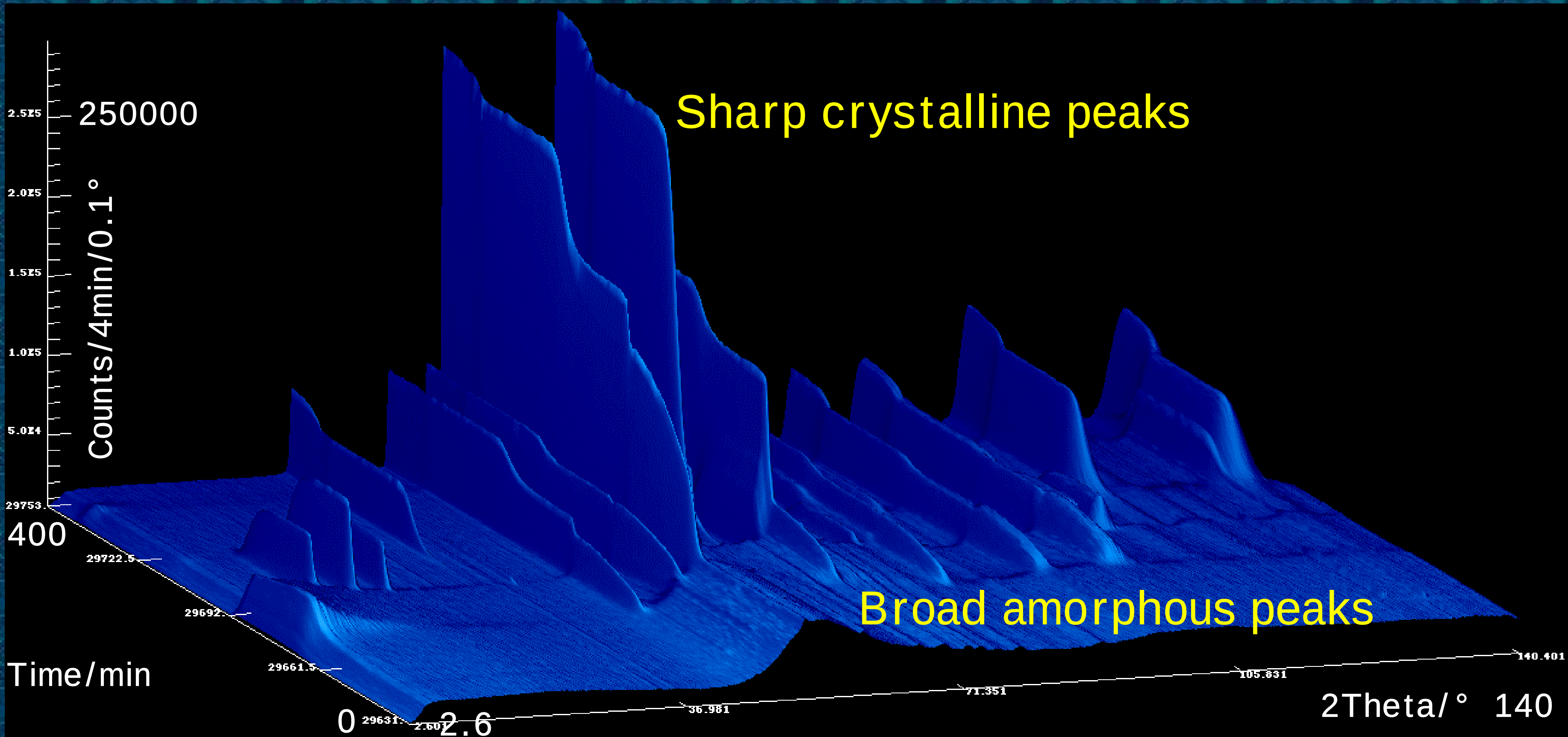
Anton Oed
Bruno Guerard
Pierre Convert
Thomas Hansen
Jacques Torregrossa

Neutron intensities are low, so large detectors are needed

Construction of a microstrip position-sensitive detector (printed circuit)

Applications of large fast detectors

Real-time Reactions - Crystallisation of amorphous alloy $Y_{67}Fe_{33}$

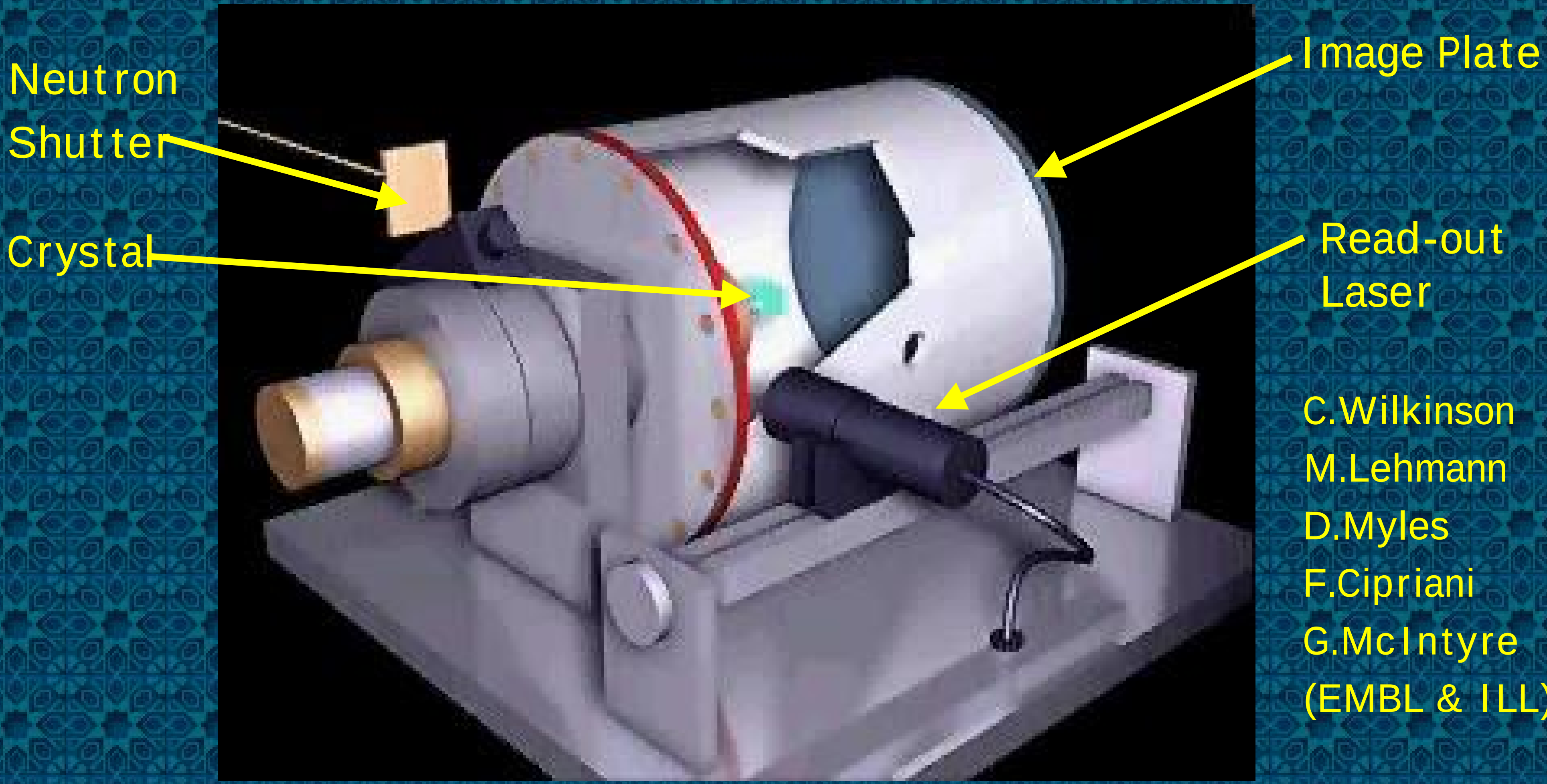


Complete diffraction pattern in minutes or seconds, scanning through temperature

R. Cywinski, S. Kilcoyne (St Andrews)

Neutron Image Plate Detectors – like photographic film

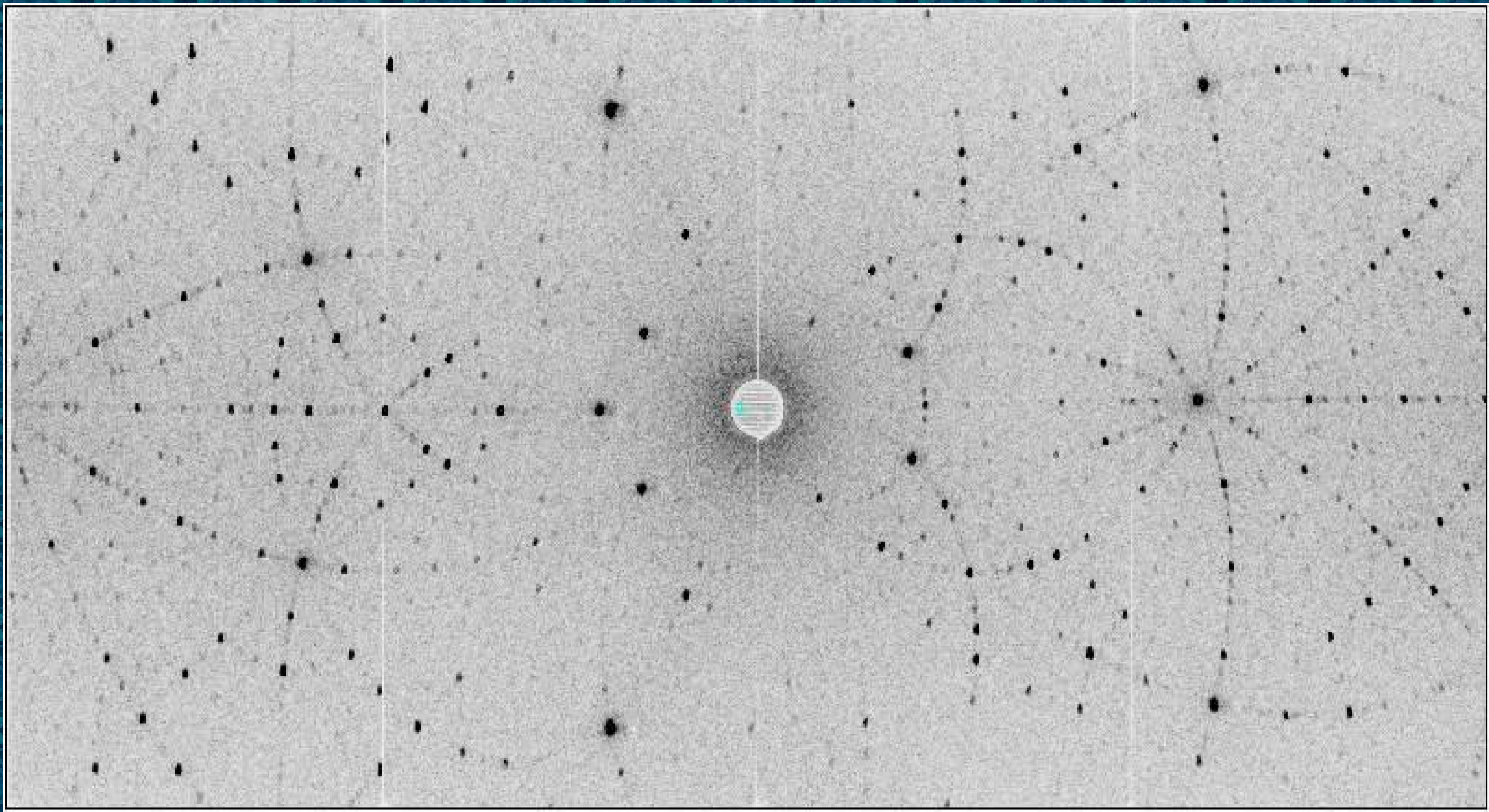
All of the scattered neutron peaks are recorded simultaneously

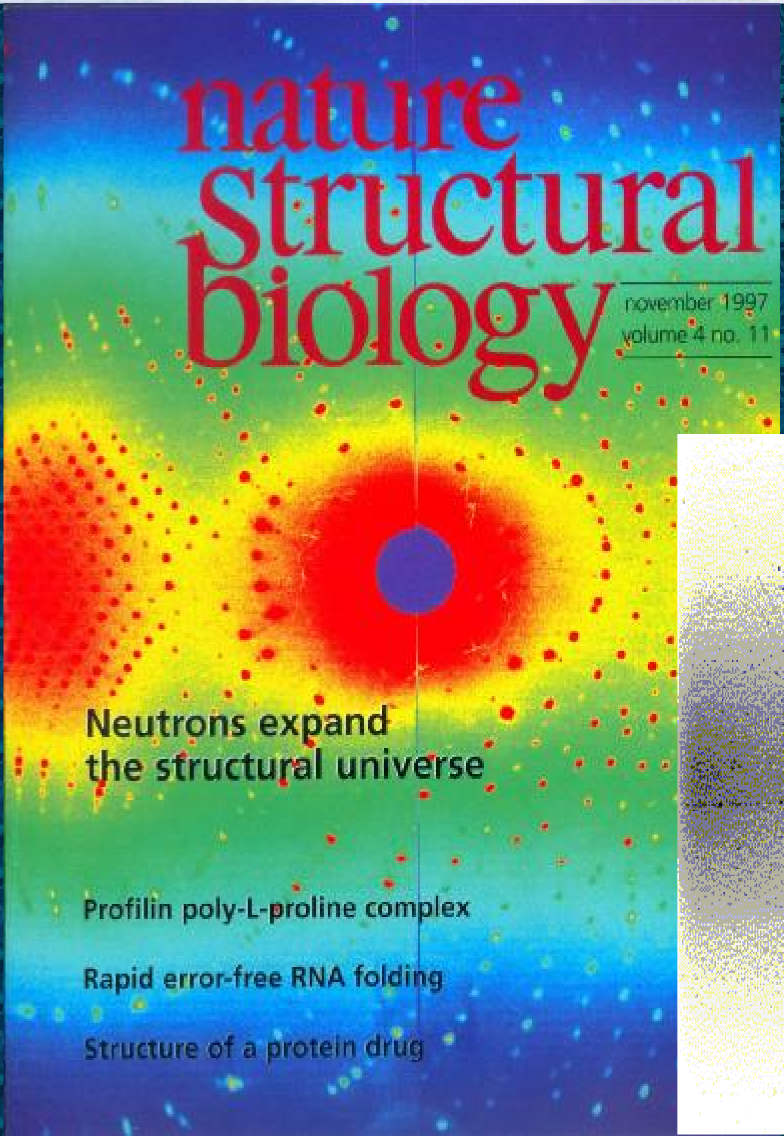


C.Wilkinson
M.Lehmann
D.Myles
F.Cipriani
G.McIntyre
(EMBL & ILL)

Neutron Image Plate & 5-fold symmetry of a quasi-crystal

All of the scattered neutron peaks are recorded simultaneously

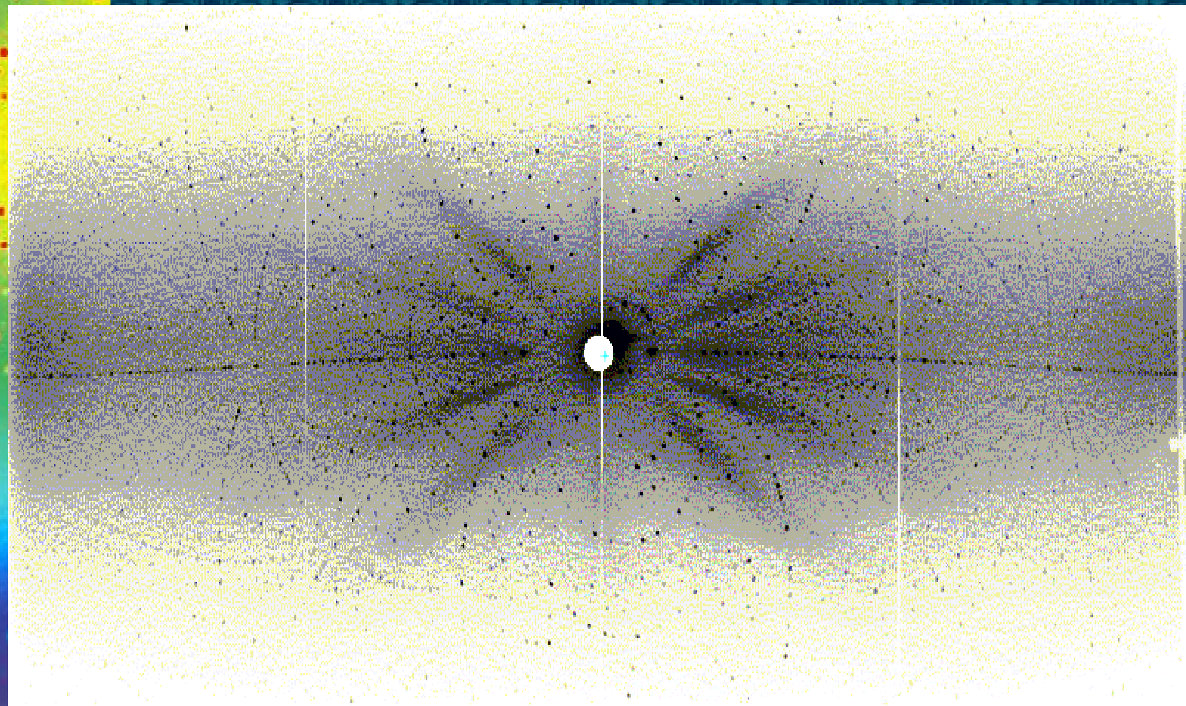




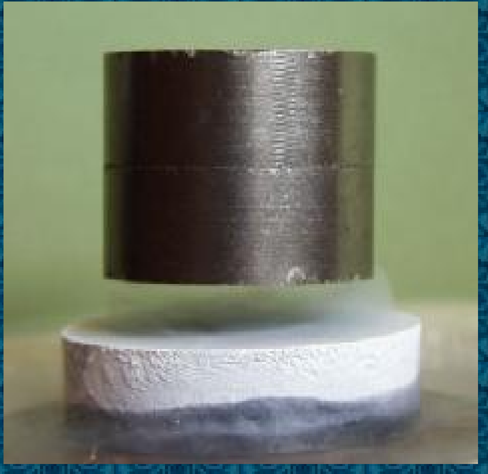
Neutron image plate detector

Large molecules and even proteins can be studied – the role of water

N.Niimura, C.Wilkinson, M.Lehmann, F.Cipriani

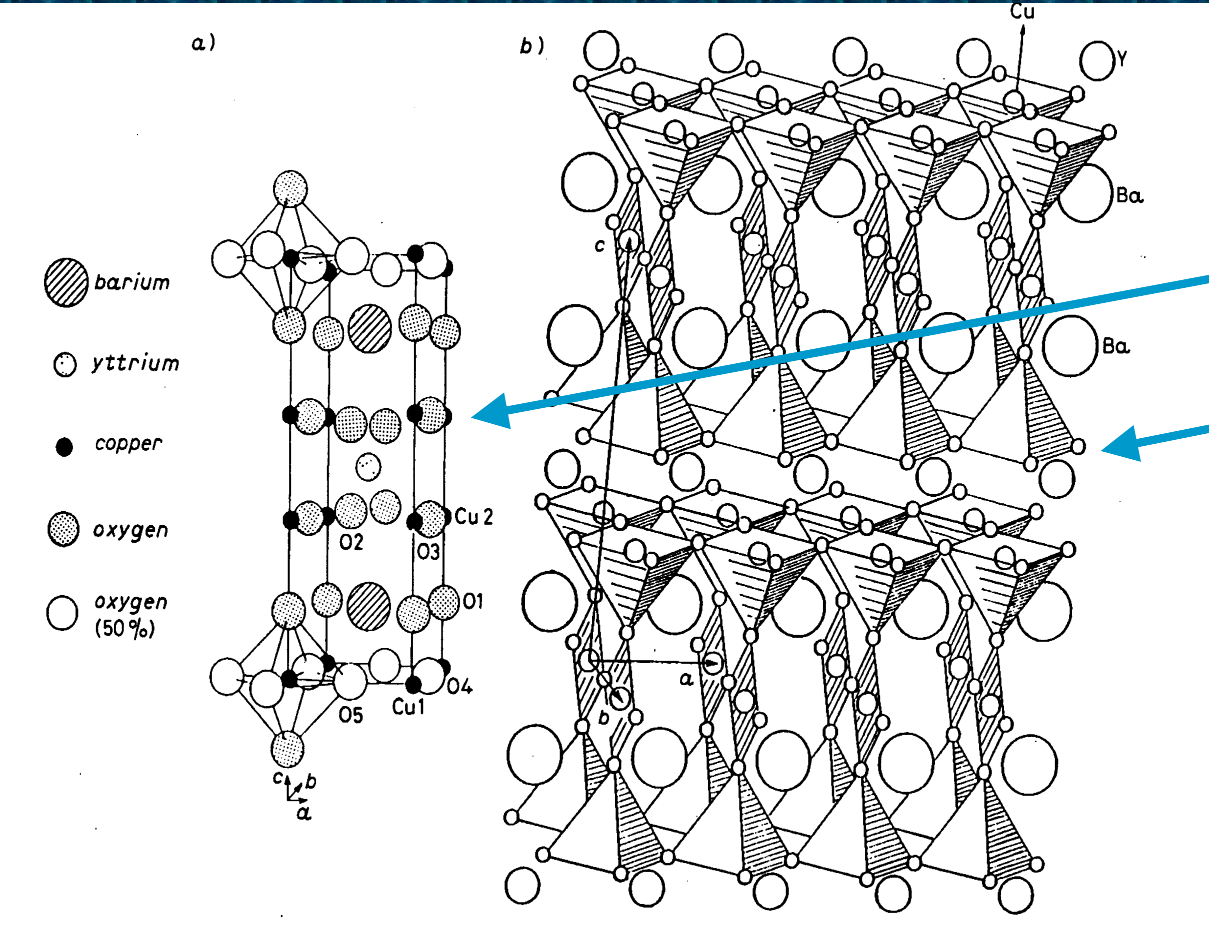


Vitamin B12 – 10,000 reflections in 8 hours from 1 mm^3 crystal



High temperature superconductors

- New magnets for medical scanners & research
- Sensitive magnetometers for mapping
- Fast connections in computer microchips
- Linear motors for high speed maglev trains



The 90K high Tc superconductor

- Left -by X-rays
- Right -by Neutrons

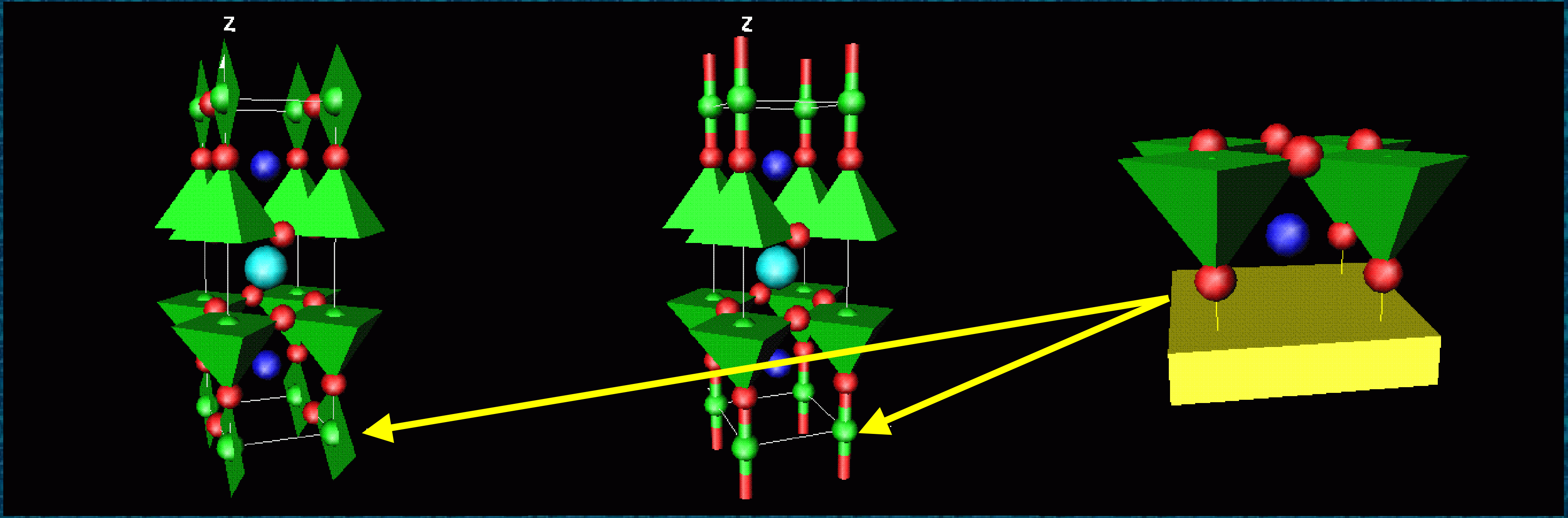
Neutrons gave new insight, important in searching for similar materials.

M. Marezio, J-J. Capponi, A. Hewat…(CNRS & ILL)

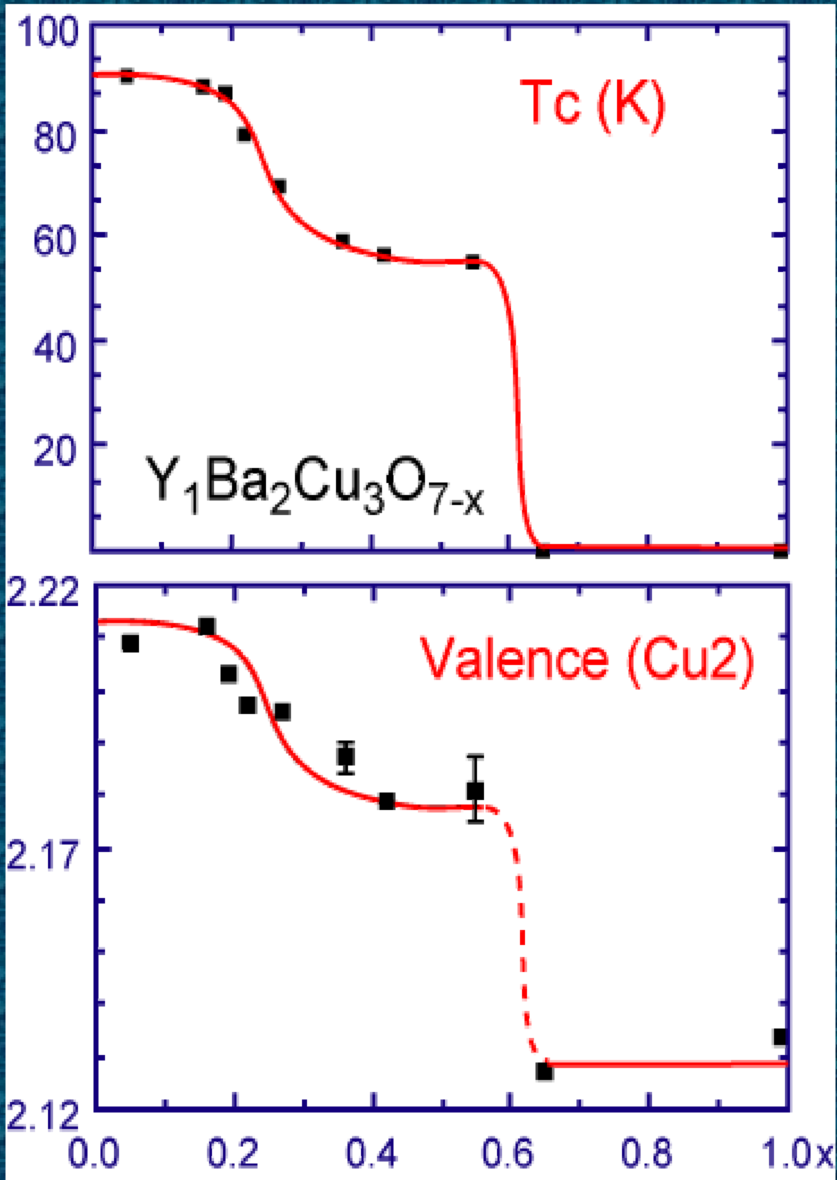
The importance of oxygen for high-Tc superconductors

Neutrons are sensitive to oxygen – "charge reservoir" concept

Superconducting $YBa_2Cu_3O_7$ Non-supercond. $YBa_2Cu_3O_6$ Charge reservoir layer



R. Cava, A. Hewat, E. Hewat, M. Marezio (Bell labs & ILL)



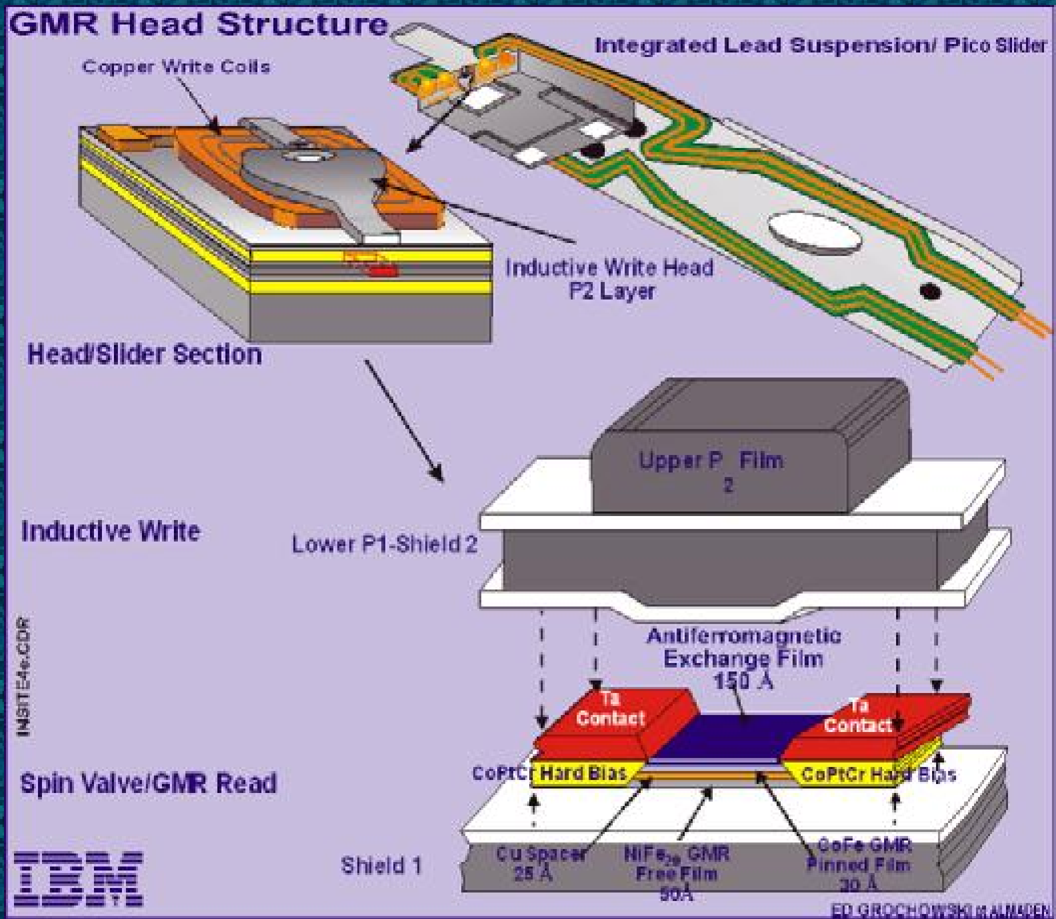
High-Tc superconductors

- Charge reservoir concept
- Tc depends on oxidation
- Imagine new charge reservoirs
- Discovery of new materials

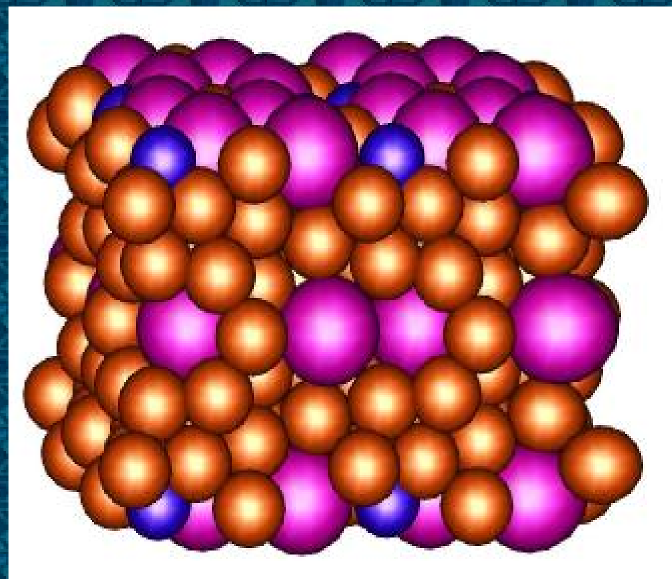
R. Cava, A. Hewat, E. Hewat, M. Marezio

Charge & magnetic order - Giant Magneto-Resistance (GMR)

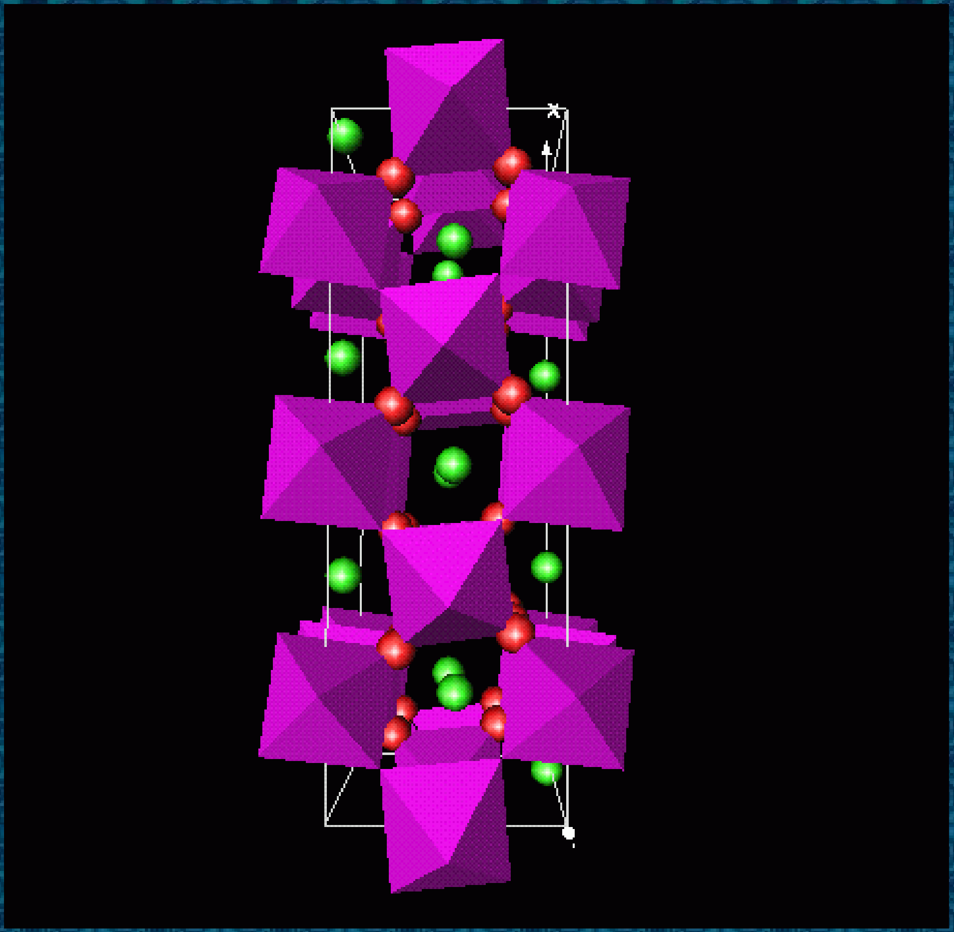
- Neutrons are important for the study of magnetic structure
- New magnetic materials for electric motors, information storage etc...



- Left – GMR computer disk
- Below – NdFeB Hard magnet



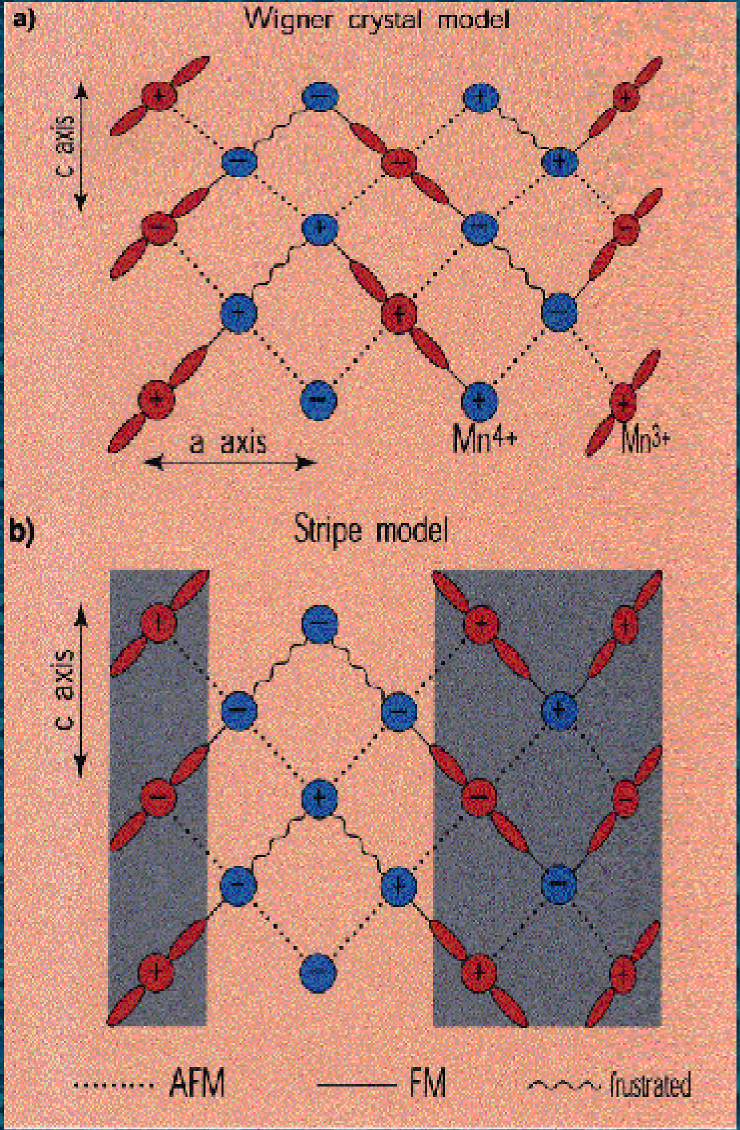
New CMR materials (Colossal MagnetoResistive) $(La,Ca)MnO_3$



- Very large changes in electrical resistivity with temperature
- mixed valence charge-ordering Mn^{3+}/Mn^{4+}
- CMR effect near room temperature

P. Radaelli, E. Suard,
M-T. Fernandez-Diaz,
J. Rodriguez, C. Ritter,
B. Ouladdiaf, R.Przenioslo
(ILL)

Neutron & Synchrotron radiation to obtain charge order



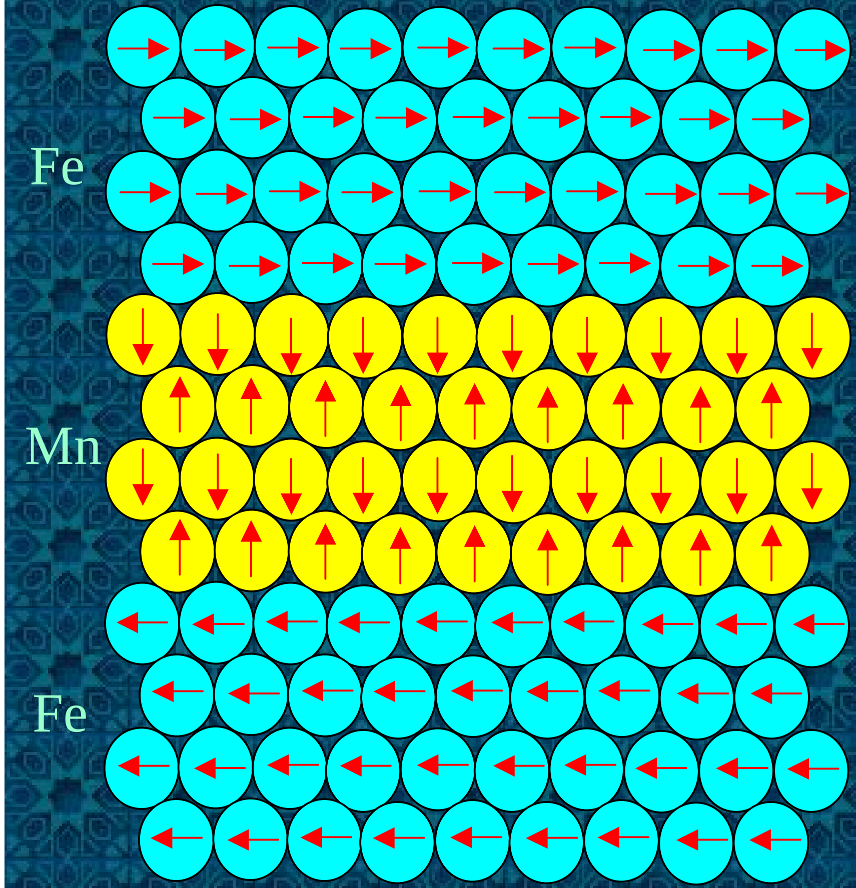
Important to decide between 2 models

a) Mn3+/Mn4+ uniformly distributed (2D Wigner model of Goodenough)

b) 1D-stripe model – this would have very important consequences for the theory of CMR materials

Stripe model excluded by the neutron and synchrotron data

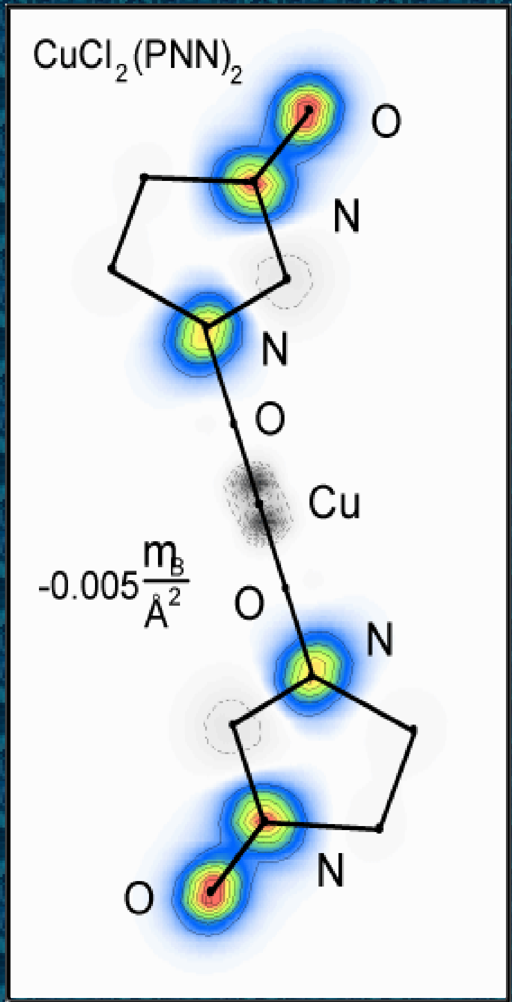
Magnetic multilayers



- Molecular Beam Epitaxy MBE allows us to build up layers on an atomic scale
- Neutrons are tiny magnets, so can be used to probe magnetic interactions between layers – neutron reflectometry
- Devices made from magnetic multilayers include “spin valves” used for computer disks and non-volatile memory

J. Goff, S. Lee, R. Ward, M. Wells, G. McIntyre (Liverpool & ILL)

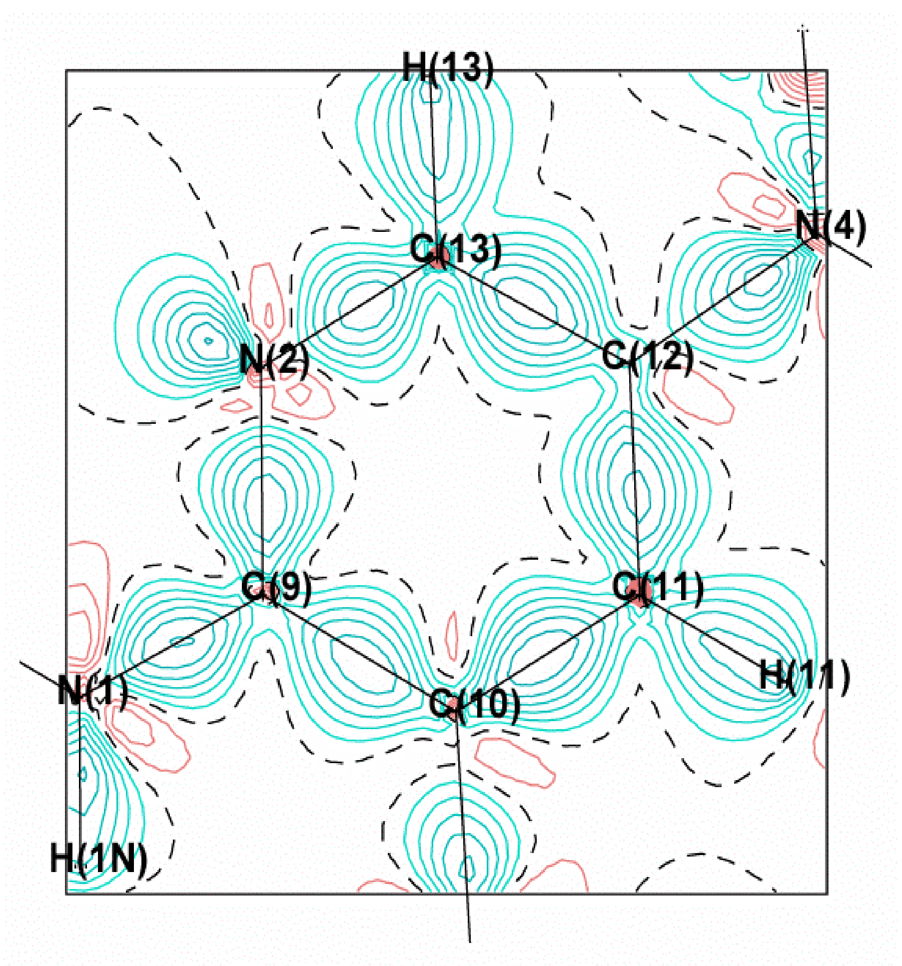
Molecular magnets



- Molecular magnets can be light, transparent, magneto-optic, bio-compatible etc...
- Neutrons are unique for mapping the magnetisation density on an atomic scale
- The first organic ferromagnet (left) - the magnetic density is on nitrogen & oxygen

E. LeLievre-Berna, E. Ressouche, J. Schweizer (ILL & CENG)

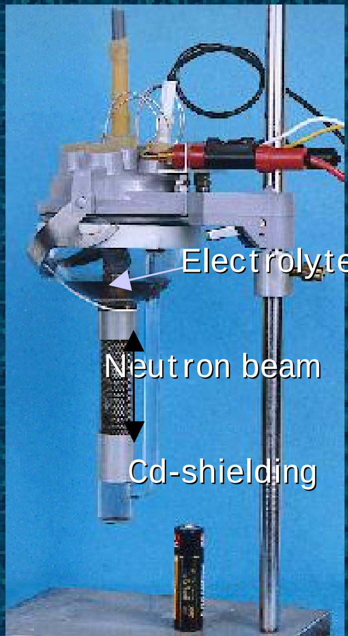
Second-harmonic organo-metallic electro-optical materials

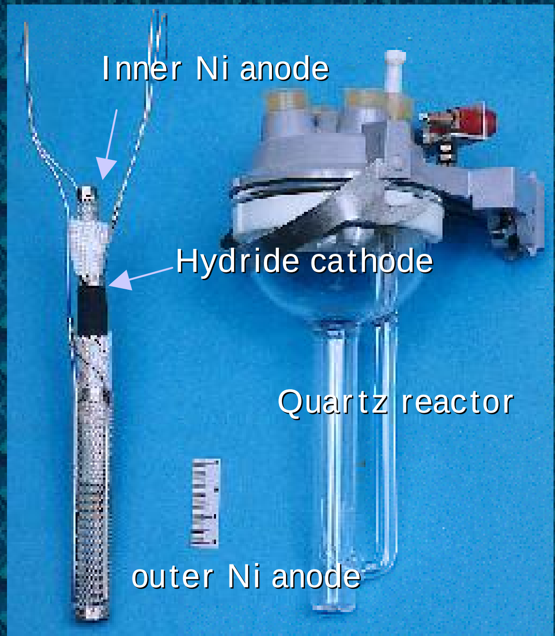


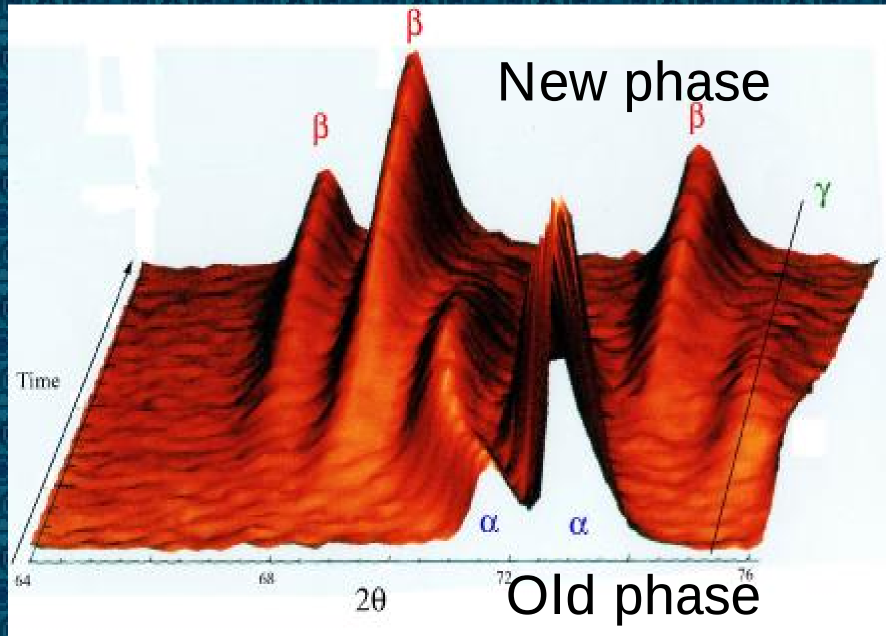
- Second-harmonic generators SHG double the frequency of light, changing a red laser beam to blue
- Shorter wavelength lasers mean more information on a CD
- SHG materials are usually inorganic, but we now have fast organic SHGs
- Neutrons can find the light hydrogen atoms, important for understanding charge transfer
- X-rays are used as well to determine the charge distribution (left)

J.M. Cole, J.A.K. Howard, G. McIntyre (Cambridge, Durham & ILL)

Electrochemistry of batteries & real-time neutron scattering







- Neutrons penetrate deep inside batteries during charge-discharge cycle
- Chemical changes due to charge-discharge can be followed in real time
- The hope is to make better batteries

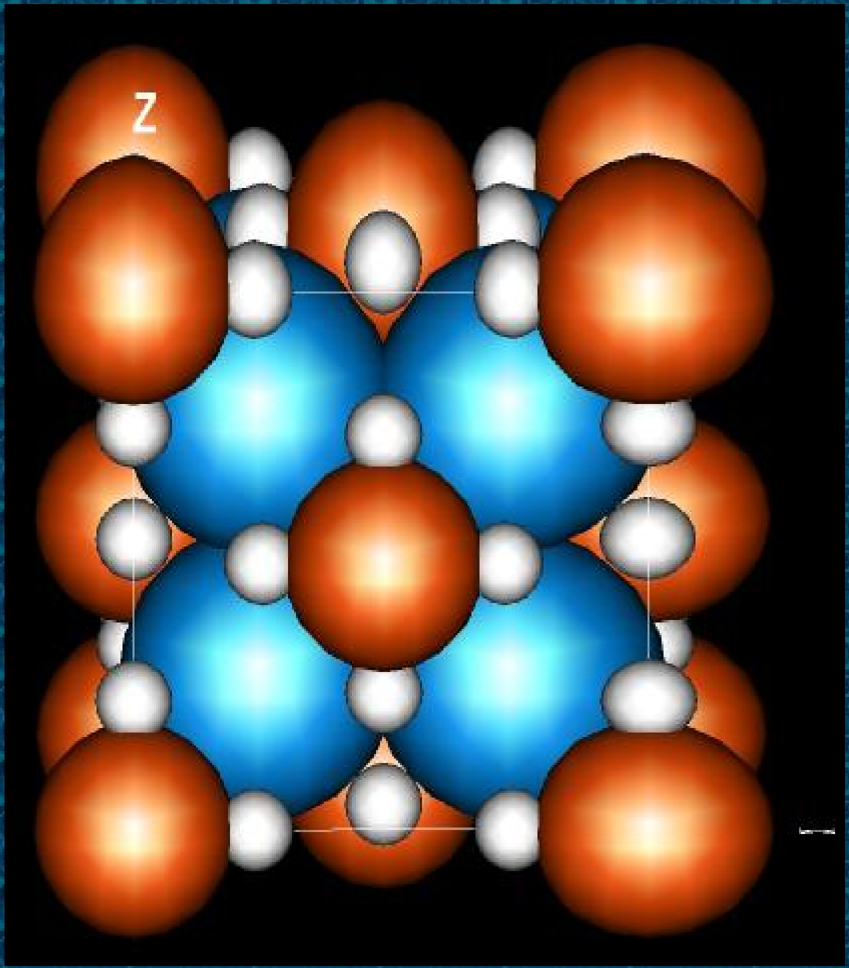
Y. Chabre, M. Latroche, M.R. Palacin,
O. Isnard, G. Rousse (CNRS, CIC-Spain + ILL)

Hydrogen storage materials

- Hydrogen is the ideal fuel
- It can be obtained from water
- It is light & doesn't pollute !
- But - explosive & difficult to store
- A new material to store hydrogen ?
- A Swiss hydrogen fueled bus. Solar electricity is used to obtain hydrogen

K. Yvon (Geneva)

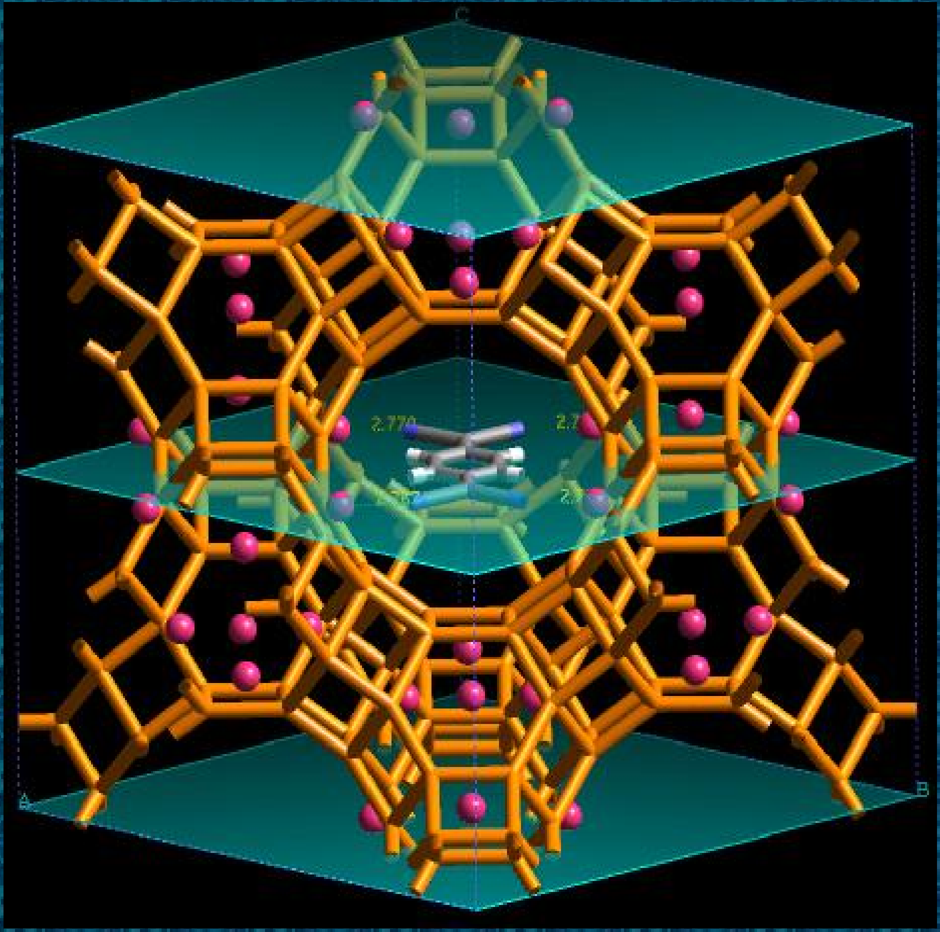
Hydrogen storage materials



- We need a material to store hydrogen
- Some materials eg Mg_2FeH_6 (left) store a higher density than liquid hydrogen
- Neutrons are used to understand how hydrogen is absorbed
- Search for better storage materials.
- The small white hydrogen atoms fill the holes between the large metal atoms

K. Yvon (Geneva)

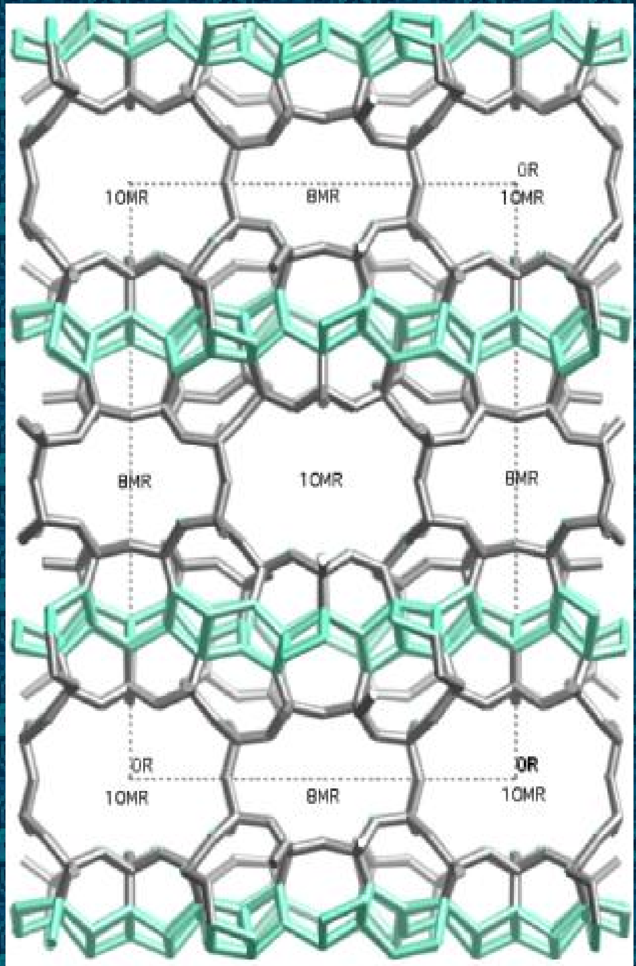
New zeolites to catalyse petro-chemical reactions



- Zeolites are very important in industry as catalysts for petro-chemicals etc
- Neutrons are used to understand how light hydrocarbon molecules interact
- Neutrons can also distinguish between silicon and aluminium in the framework
- A small organic molecule trapped inside the pore of NaY-zeolite.

C. Baehtz, H. Fuess (Darmstadt)

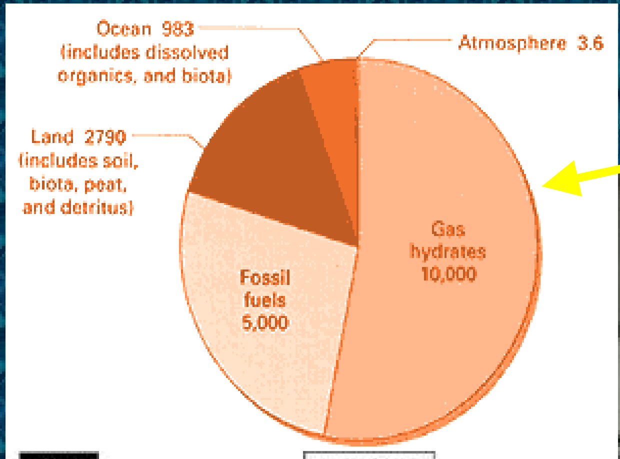
Molecular sieves and ion exchangers

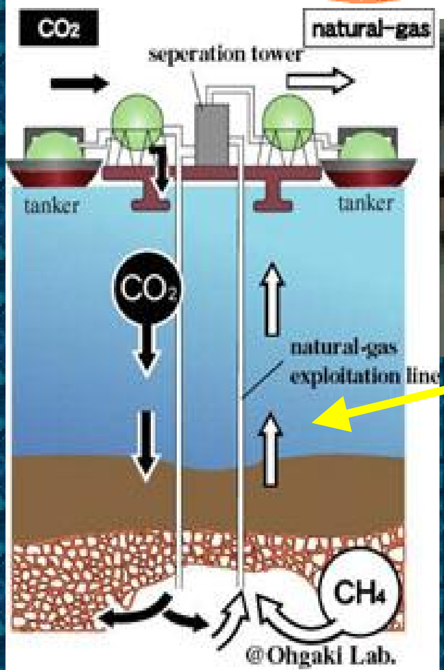


- Ion exchangers can remove toxic metals from the environment
- New types of zeolite ion-exchangers are needed to trap specific elements
- Neutrons and synchrotron radiation are used to understand ion exchange
- RUB29, a new lithium zeolite for cleaning up radioactive caesium

J.B.Parise, S-H.Park, A.Tripathi, T.Nenoff, M.Nymann (SUNY & SANDIA)

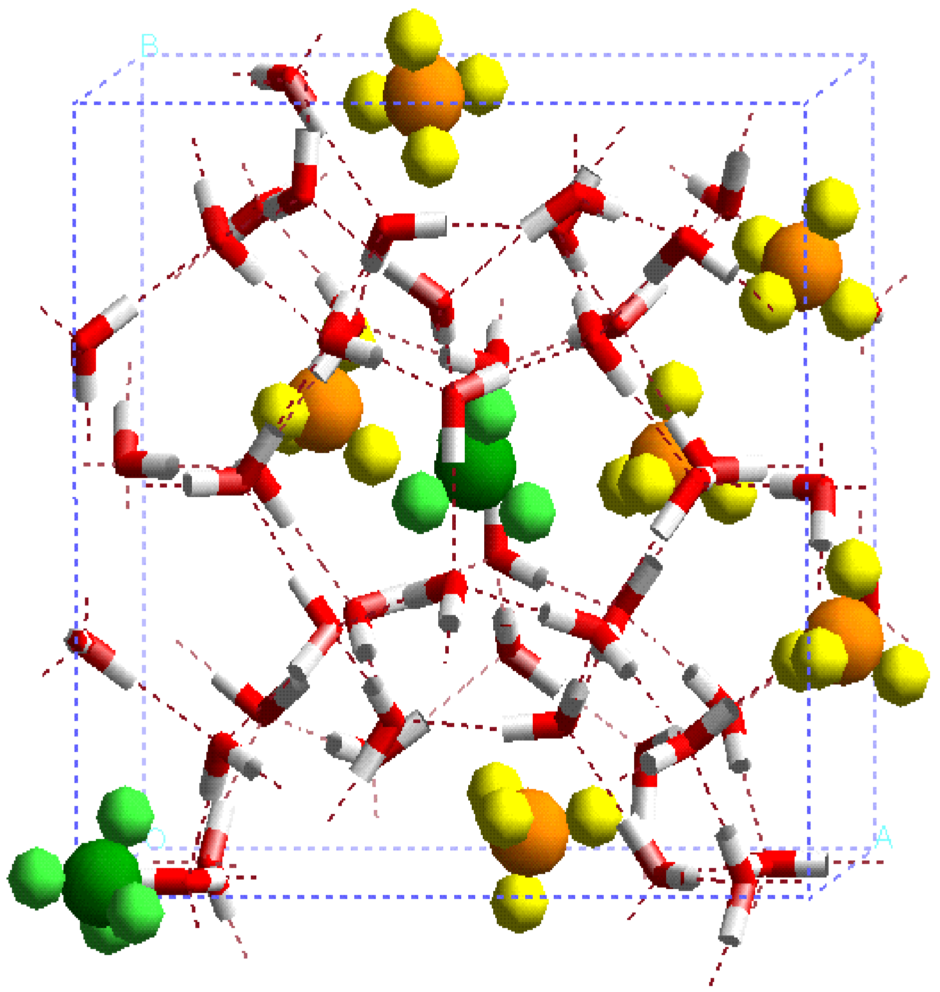
Clathrates, new gas hydrate fuel from the ocean





- Most hydrocarbons are locked in water cages at the bottom of the oceans
- These gas hydrates can be used as fuel
- A closed fuel cycle – extraction of methane and storage of CO2 in the deep ocean
- Neutrons are needed to learn more about these strange “clathrates”

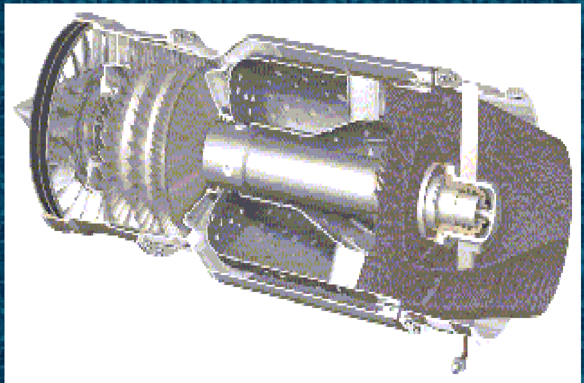
Clathrates, new gas hydrate fuel from the ocean

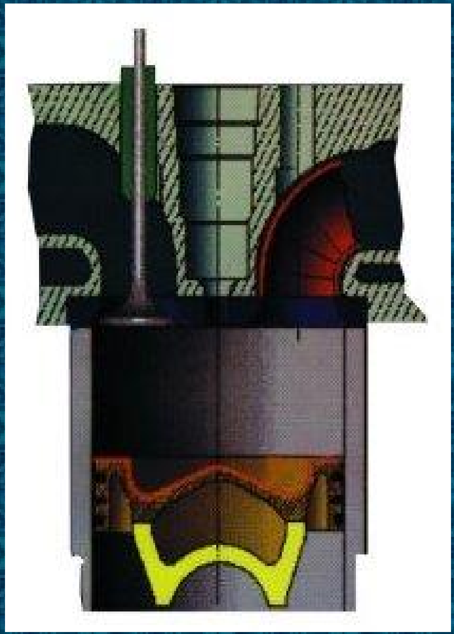


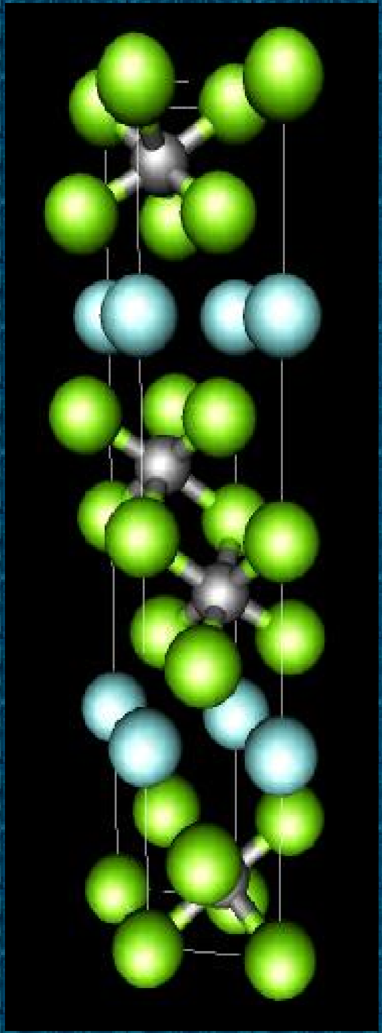
- Clathrates consist of molecular cages that can trap methane (spheres)
- Neutrons are important – they scatter strongly from the light methane atoms
- Compressibility was studied, to help with seismic searches for clathrates

B.Chazallon, A.Klaproth, D.Staykova, W.Kuhs (Göttingen)

New ceramics to replace metals in engineering components



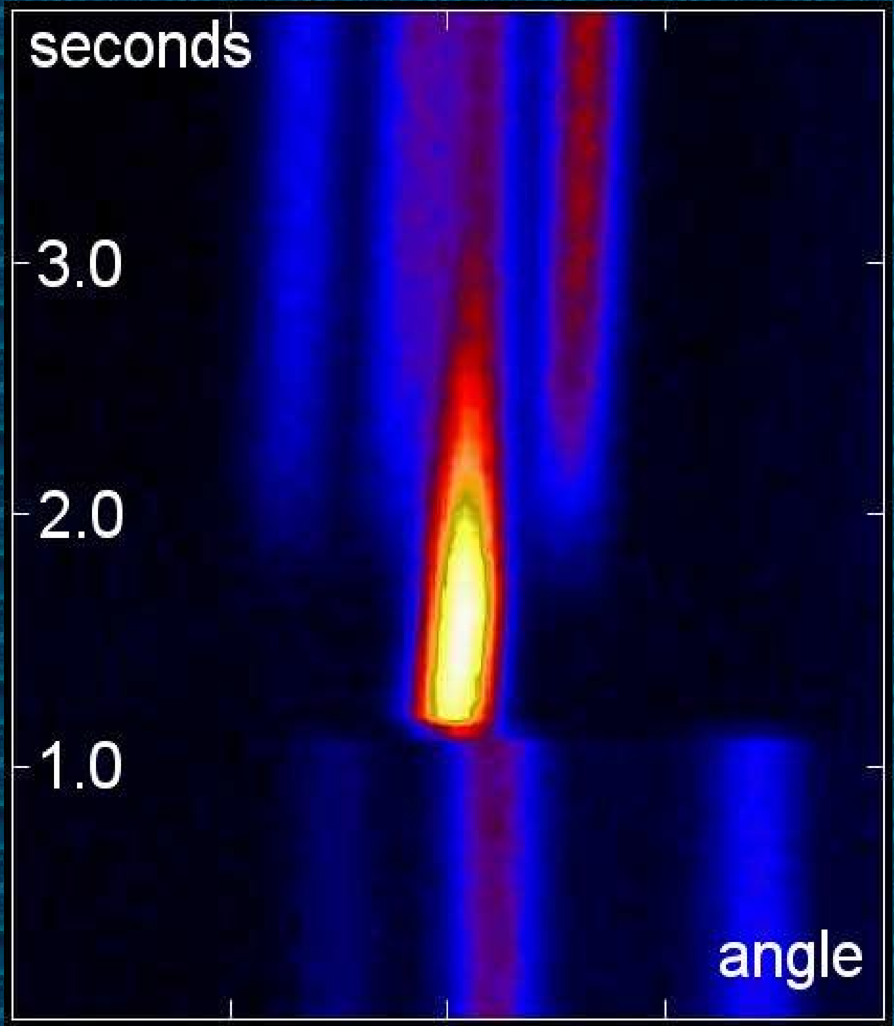




- Titanium silicon carbide Ti_3SiC_2 conducts heat and electricity
- It is tough, easily machinable
- Potential engineering applications as a light replacement for metals
- BUT, difficult to prepare pure
- Neutron diffraction has been used to study high temperature self propagating synthesis – SHS

D. Riley, E. Kisi (Newcastle, Aust.)

New ceramics to replace metals in engineering components

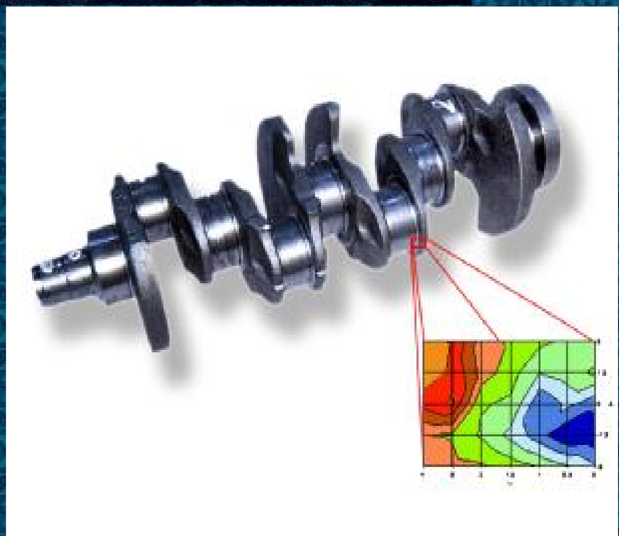


- The explosive SHS reaction was studied in real time with neutrons
- The reaction is exothermic, & heats the sample to 2200ºC in <1 sec
- The complete diffraction pattern (left) is collected at 500 ms intervals
- Knowledge of the SHS process allows us to prepare a pure Ti_3SiC_2 product

D. Riley, E. Kisi (Newcastle, Aust.)

Measuring stresses deep inside engineering components

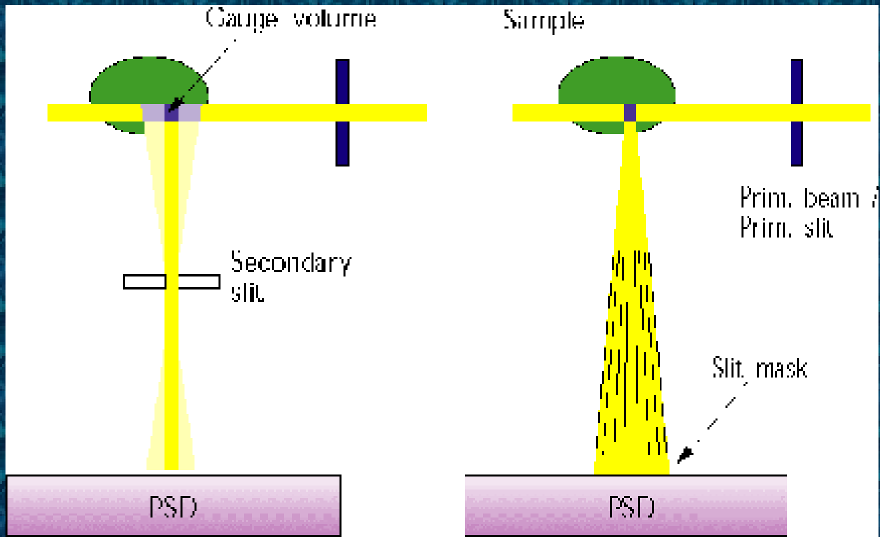
- Tensile stress can produce cracks
- Compressive stress toughens materials
- Neutrons can penetrate deep inside materials (~10cm) and measure stress by changes in atom spacings



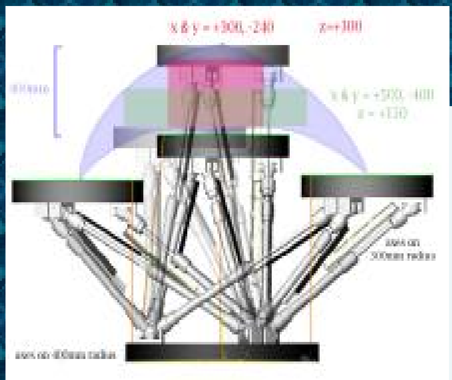
- The compressive stress (blue) deep inside a VW crankshaft
- Design of stronger, lighter engines

T. Pirling, G. Bruno (ILL & Manchester)

Measuring stresses deep inside engineering components



- The neutron beam is collimated to a $1mm^3$ “gauge volume” of measurement
- The scattered peak is measured on a position-sensitive detector (PSD)
- Small shifts in peak positions map the strain as the sample is scanned



- Very large engineering components (1 tonne) can be scanned using a “hexapod” platform (similar to the platform of an aircraft flight simulator)

T. Pirling, G. Bruno (ILL & Manchester)