Neutron Scattering: The Future

CLRC

Andrew Taylor

Director ISIS

Workshop on Neutron Detectors for Spallation Neutron Sources

BROOKHAVEN NATIONAL LABORATORY

25 September 1998

Outline

- **Neutron Sources & Neutron Science**
  - Why we build neutron sources

- **Pulsed Spallation Sources**
  - The way forward

- **Scientific & Industrial Impact**
  - Excellence and Relevance

- **The Need for Next Generation Sources**

ess european spallation source

USA *Europe* Japan

1994 Nobel Prize for Physics

B. N. Brockhouse

C G Shull

Pioneering contributions to the development of neutron scattering techniques for studies of condensed matter

Where atoms 'are'
What atoms 'do'

Big Facilities for Small Science

Tools which help us understand the world around us at a microscopic level

Where atoms and molecules *'are'*

What atoms and molecules *'do'*

No one experiment

Used by thousands of scientists each year as part of their research programmes in

Biology	***Engineering***
Chemistry	***Materials Science***
Physics	***Earth Science***

Neutrons -- an Ideal Probe for Condensed Matter Science

- **Neutron wavelength and energy appropriate for condensed state**
  - **structure and dynamics**
- **Neutron cross-section**
  - **isotopic dependence H - D contrast**
  - **nuclear form factor**
- **Magnetic moment μ**
  - **magnetic order and excitations**
- **Weak probe**
  - **theoretical interpretation**
  - **molecular dynamics**
- **Highly penetrating**
  - **bulk probe**
  - **complex sample environments**

Illustrations of the advantages of neutrons
(Slides not included)

- **Neutron wavelength and energy**

Neutron-Photon dispersion
S(Q,w) of random network glass

- **Neutron cross-section**

Nuclear and Magnetic scattering lengths
H/D contrast and applications to surfactants

- **Magnetic moment μ & Weak probe**

Soin waves
Comparisons with theory & MD simulations

- **Highly penetrating**

Residual stress in bulk engineering components
Jet engine turbine blades
High pressure diffraction (up to 300kbar) and applications to the highest Tc mercury superconductors

Why neutrons ?

- *wavelength - energy perfect match*
- *unique cross-section*
- *magnetic moment*
- *comparison with theory*
- *penetrating power*

What do we need - more flux !

Present day sources are about as bright as a candle viewed at 10m !

Pulsed Neutron Sources

Neutrons are an ideal probe

but

Present day neutron sources are flux limited by heat dissipation

- Reactor based sources
  Fission - 190 MeV/n

- Accelerator based sources
  Spallation - 30 MeV/n
  Naturally pulsed ~1μs

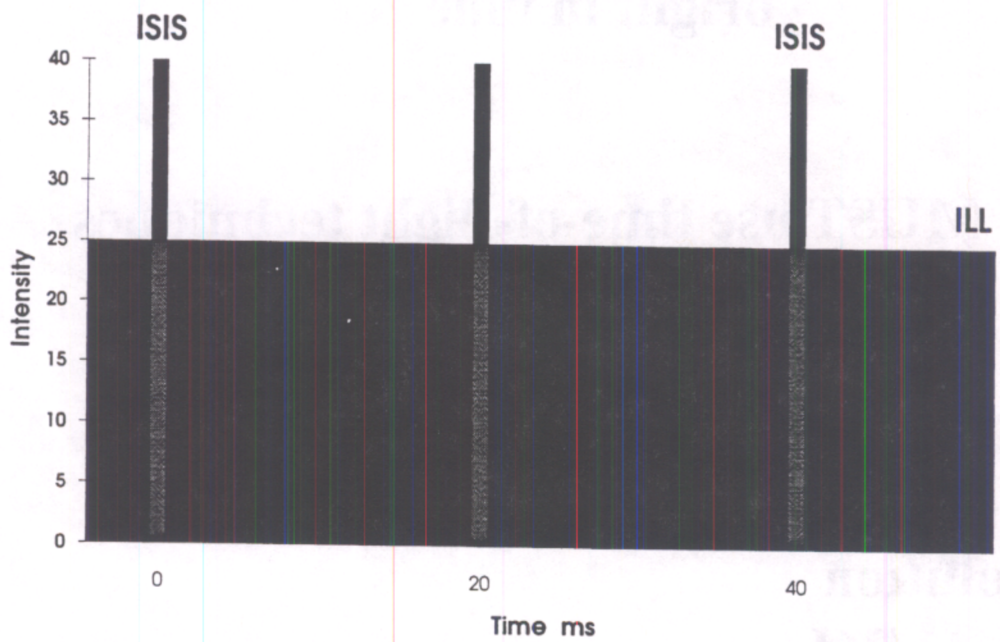
(Pulsed reactors have broad (~200μs) time structure)

ISIS (200kW) ↔ ILL (58MW)

Pulsed Neutron Sources

vs

Steady State Sources



$\Delta t \sim 1\ \mu s$

$\tau \sim 20$ ms

ISIS (200kW) ←→ ILL (58MW)

Pulsed Neutron Sources

- Time average flux low
  - heat dissipation low

- Peak flux high
  - bright in time

- ➔ MUST use time-of-flight techniques

$t = 252\lambda L$; $\Delta t \sim 7\lambda$ (μs-m-Å)

Resolution

$\Delta t/t = 1/36L$

= very good

(eg 0.3% at 10m; 0.03% at 100 m)

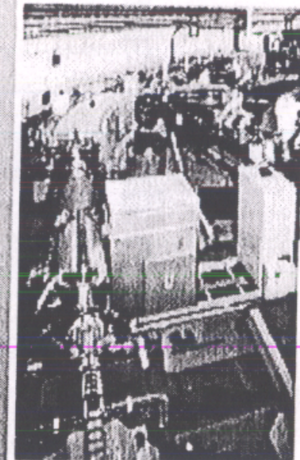
Braggs Law $\lambda = 2d \sin\theta$

$$\mathbf{t} \ \alpha \ \mathbf{d} \sin\theta \ L$$

Accelerator Driven Pulsed Spallation Sources

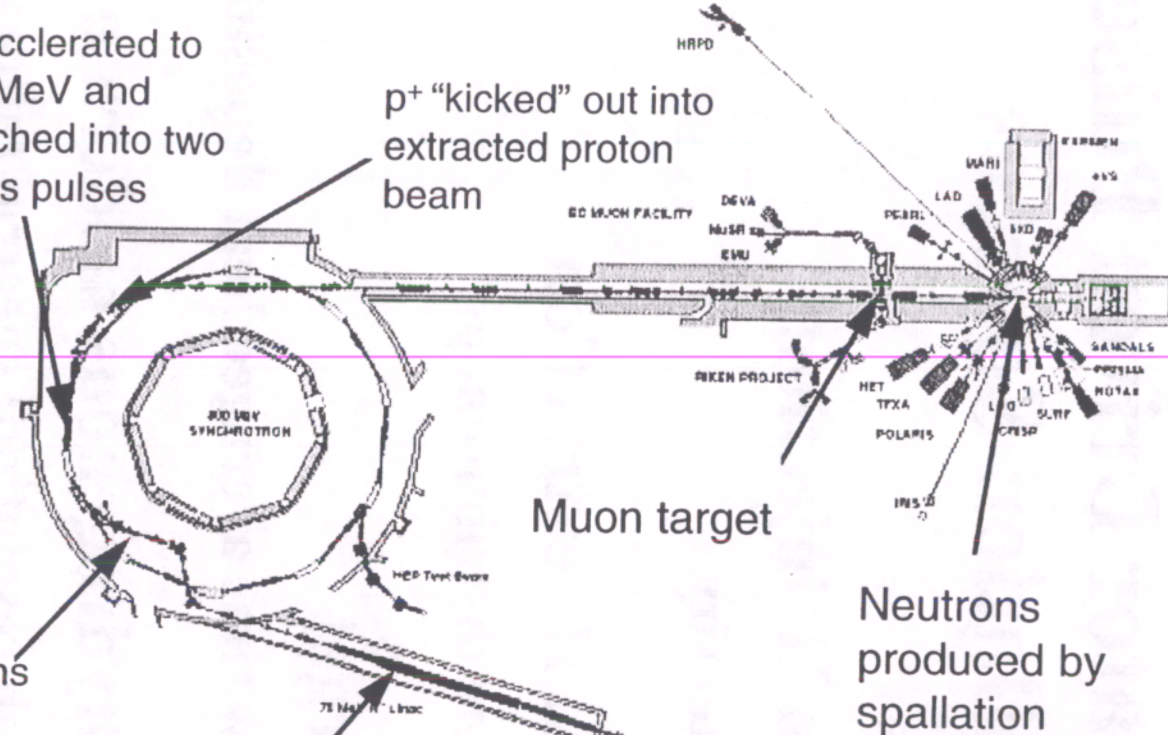
- Multi-turn H^- injection
  - intensity
- Single turn H^+ extraction
  - time distribution μs
- High Z target
  - low time averaged heat deposition
- Compact hydrogenous moderators
  - high resolution; spectral tailoring
- Time-of-flight instrumentation
  - area detectors & high data rate

Producing Neutrons and Muons



p+ acclerated to 800MeV and bunched into two 0.3μs pulses

p+ "kicked" out into extracted proton beam

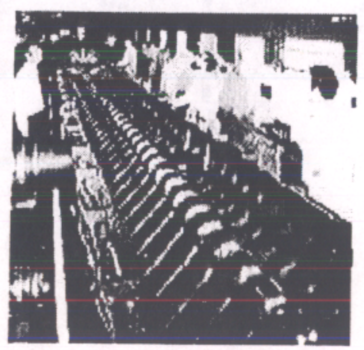


Muon target

Neutrons produced by spallation

Stripped of electrons

H⁻ ⇨ p+



H⁻ ions produced at -665kV

H⁻ ions accelerated to 70MeV in LINAC

ISIS

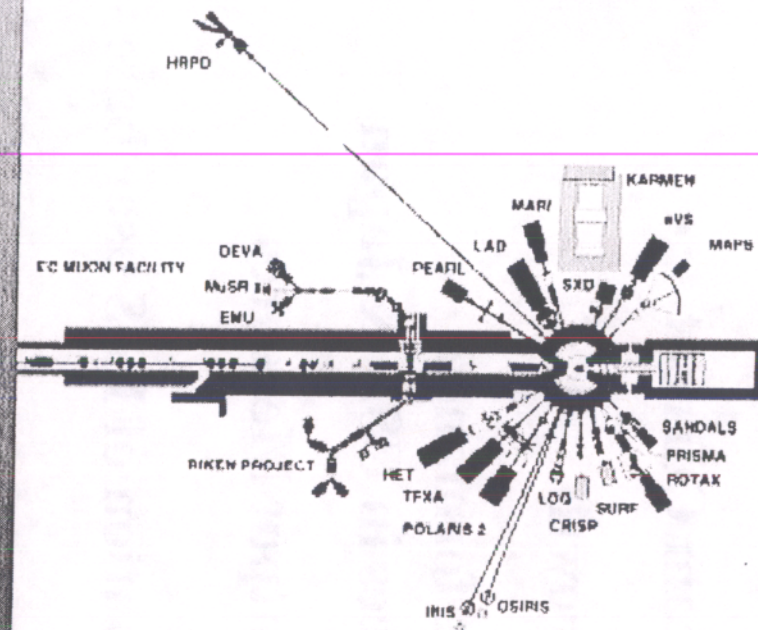
Slides of the ISIS Facility (not included)

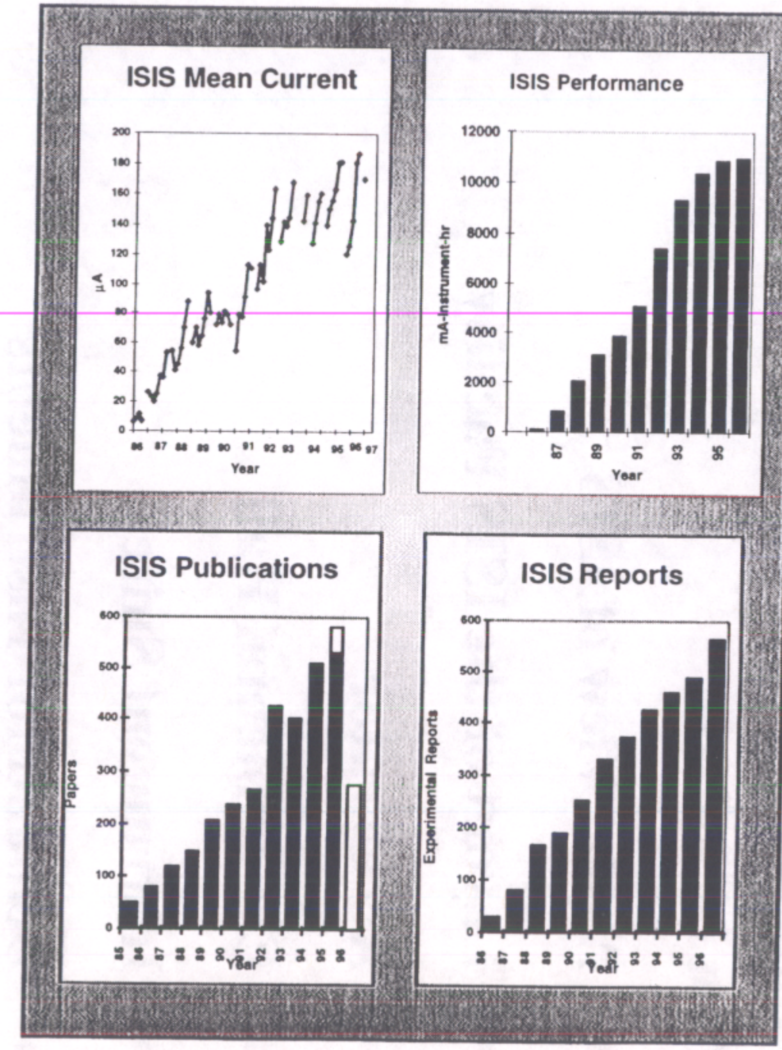
- **Aerial View of ISIS**
- **Layout of the ISIS Facility**
- **Accelerator**
- **Experimental Hall**
- **Instrument Suite**
- **Demand for Instruments**
- **ISIS Beam Current**
- **ISIS Growth**
- **ISIS Performance cf sources in USA & Japan**
- **ISIS Output Measures**

Age distribution of ISIS user base

User Community in Europe - from ESS Vol 1

ISIS Status and Performance

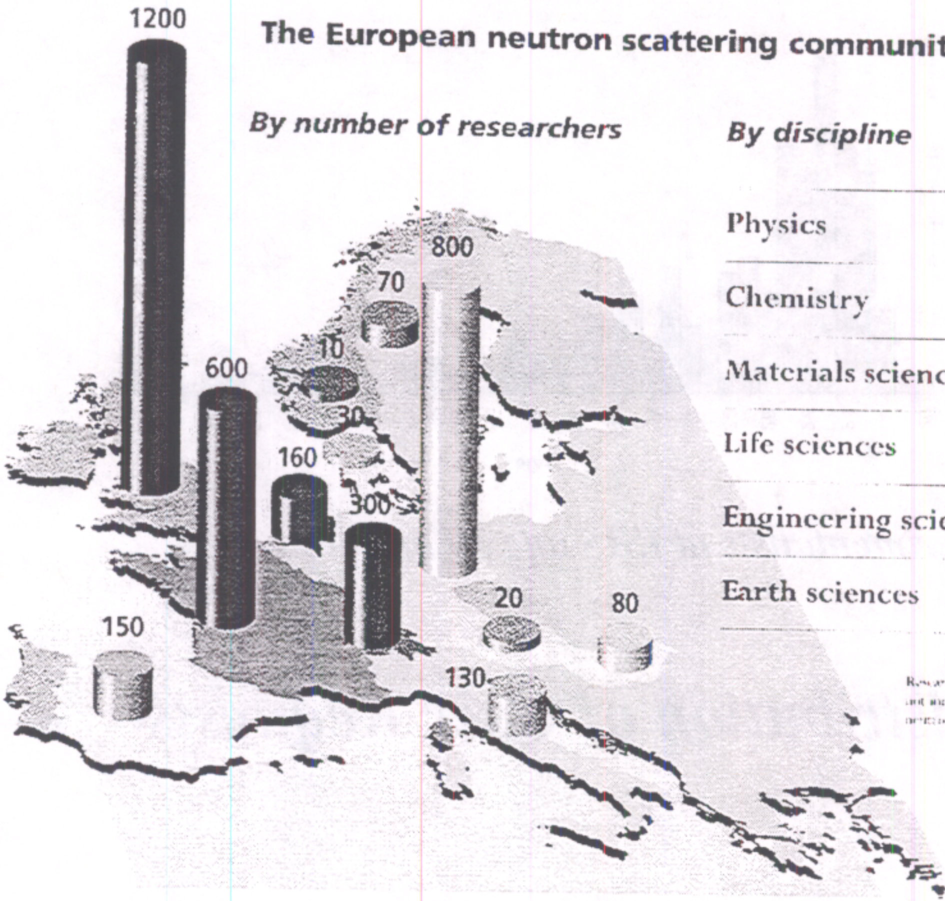




User Community in Europe

The European neutron scattering community

By number of researchers



By discipline

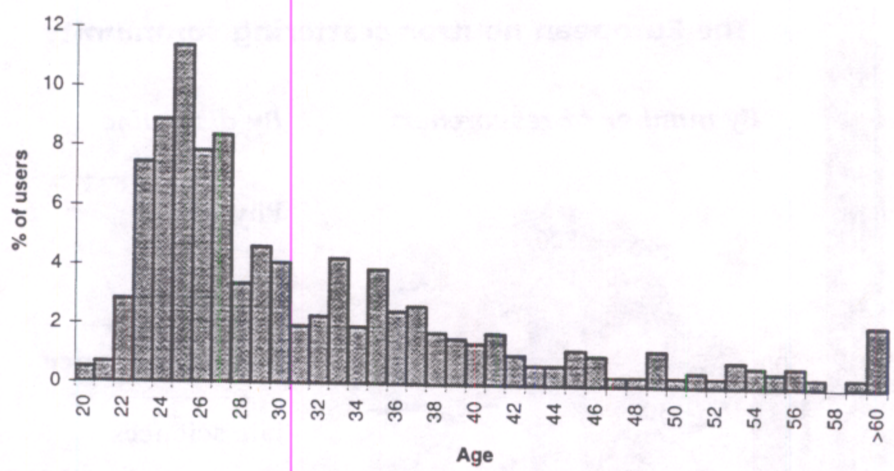
Physics	46%
Chemistry	26%
Materials science	20%
Life sciences	4%
Engineering sciences	3%
Earth sciences	1%

Source: ENSA Survey

Researchers in other European countries not included in this survey also use neutron facilities.

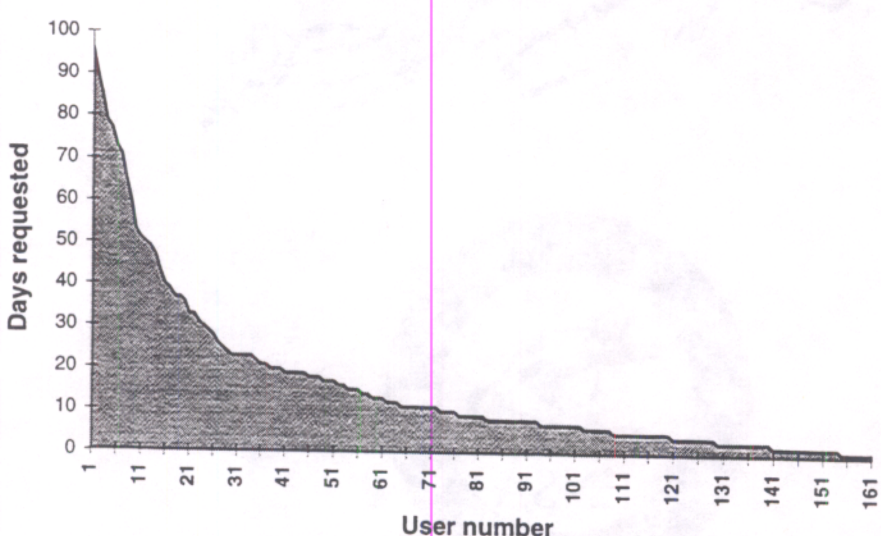
ISIS User Base

Age Distribution



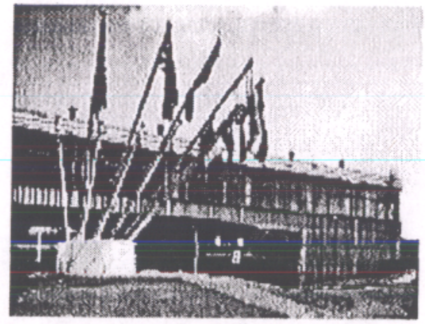
60% of Experimentalists at ISIS age 30 or younger

Distribution of User Requests

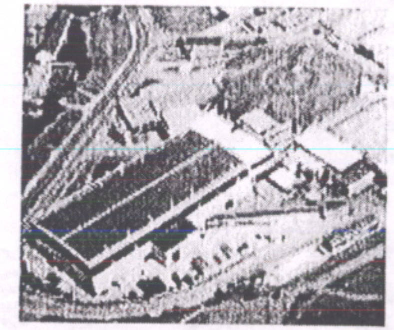


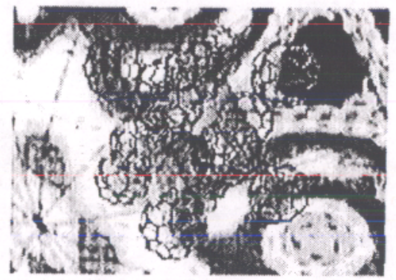
Very broad range : 90 days/year to 1 day /year

A World Centre for Condensed Matter Research

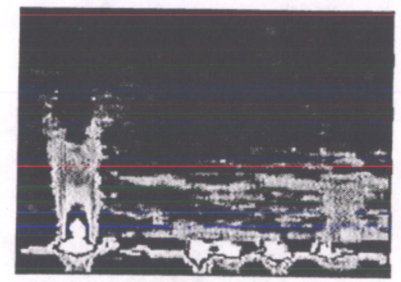


ISIS

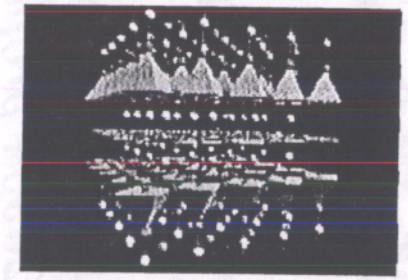




Chemistry

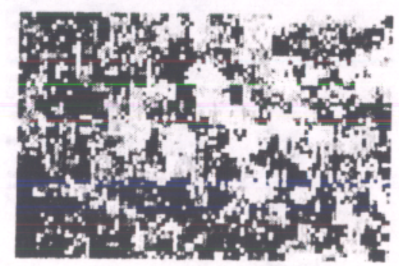


Physics

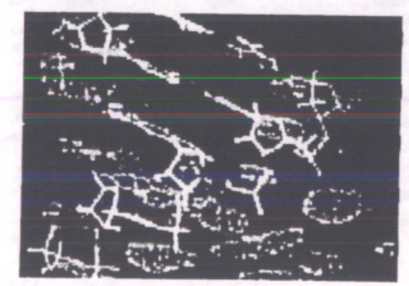


Materials Science

Engineering



Geology



Biology

ISIS

Science at the ISIS Facility

Excellence and Relevance

Over 600 experiments per year selected by peer review from the 2000+ proposals

Mostly UK HEIs & Industry but 25% 'overseas'

- **Basic**
  - unbound spinons
  - fullerene and fullerides
  - solvation
- **Strategic**
  - superconductors
  - zeolites
  - surfactants
- **Applied**
  - GMR and spin valves
  - engineering stress
  - green refrigerants

Illustrations
(Slides not included)

Basic

Structure of fullerene; quality data from world's highest resolution neutron powder diffractometer; superconducting and insulating fullerides

Applied

Lap-top computer - contributions of neutron scattering to
- liquid crystal display technology
- hard disk: magnetic thin films
giant magnetoresistance
- casing - polymers & recycling issues
- batteries

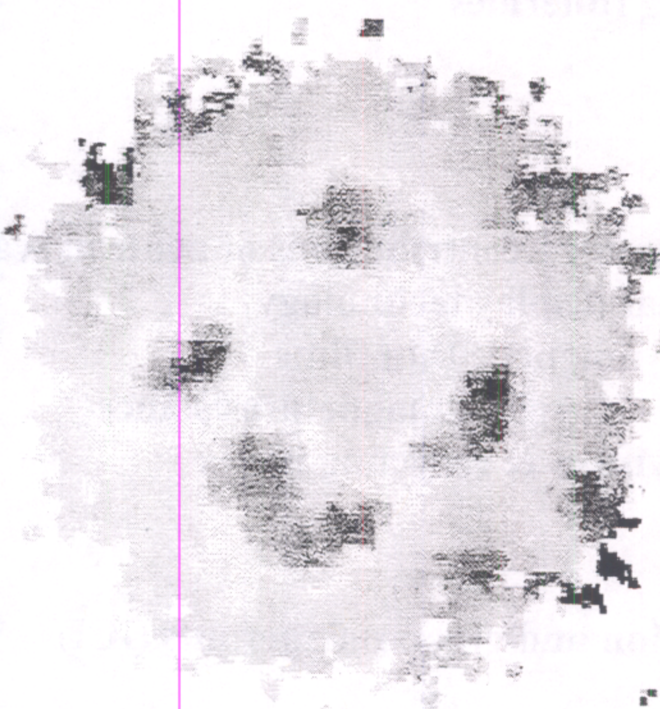
Ozone depletion and green refrigerants (ICI)

Basic / Strategic / Applied

Understanding the behaviour of spins in 1-D quantum systems; high temperature superconductors and colossal magnetoresistance materials

Science at the ISIS Facility

ISIS 98



600 Experimental Reports / year

450 Publications / year

£40k per publication

Disadvantages of Pulsed Spallation Source

- **Capture Flux is Low** — **TRUE**
  - isotope production
- **Limited Experience** — **But growing !**
- **Poor for**
  - Cold Neutrons — **FALSE**
  - High Resolution Spectroscopy — **FALSE**
  - Magnetic Diffraction — **FALSE**
  - Excitations in Single Crystals — **FALSE**

Advantages of a Pulsed Spallation Source

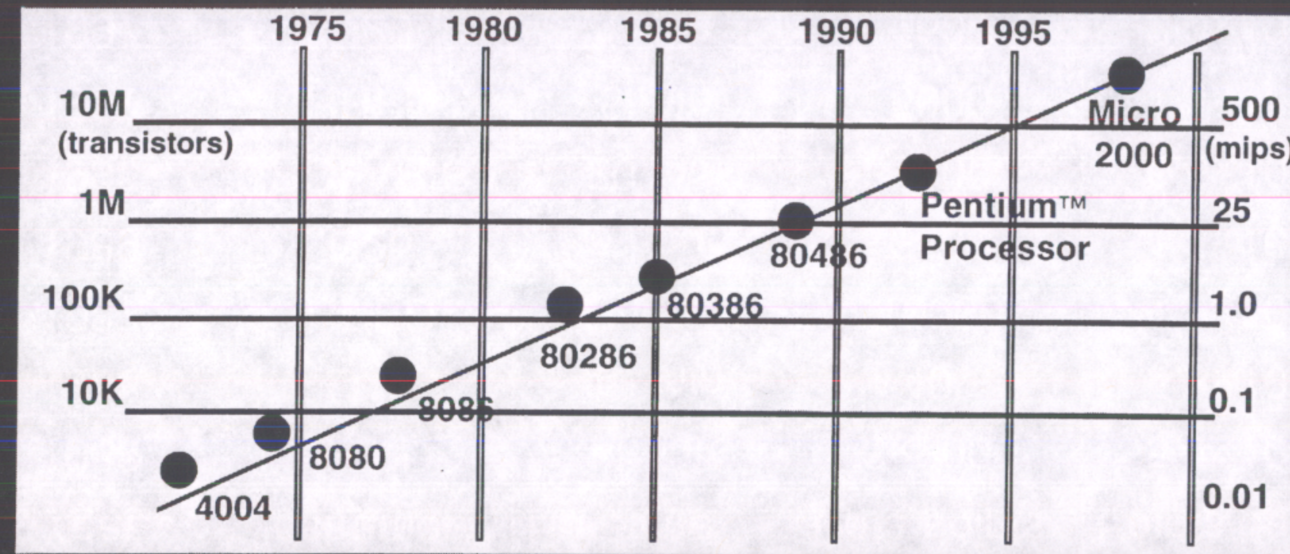
- ***Wide spectral range*** **-μeV to eV**
- ***Fixed Geometry*** **-extreme environment**
- ***High Brightness and Excellent S/N*** **- small samples**
- ***High Intrinsic Resolution*** **- subtle effects**
- ***Wide Dynamic Range*** **- whole picture**

*****Pixel Power*****

Gordon Moore (Intel) 1965

Moore's Law

Each new chip contained roughly twice as much capacity as its predecessor, and each chip was released within 18-24 months of the previous chip.



Machrone's Law

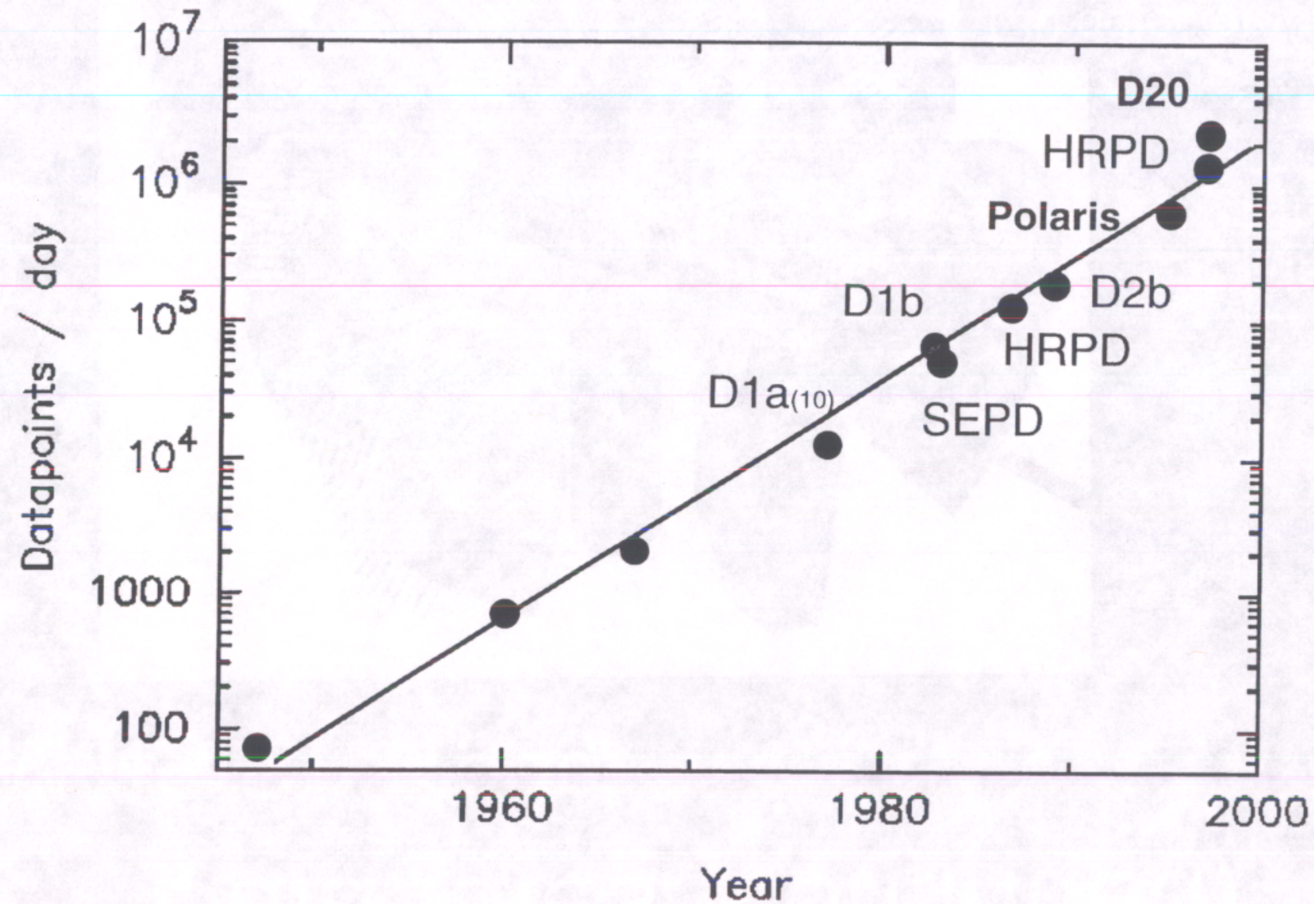
"Gordon Moore just plain got it right . . .
Moore's Law has also given rise to Machrone's Law, which was true for many years, which is that the machine you want always costs $5,000." -Bill Machrone

Rock's Law

"A very small addendum to Moore's Law is Rock's Law which says that the cost of capital equipment to build semiconductors will double every four years."

Data rates

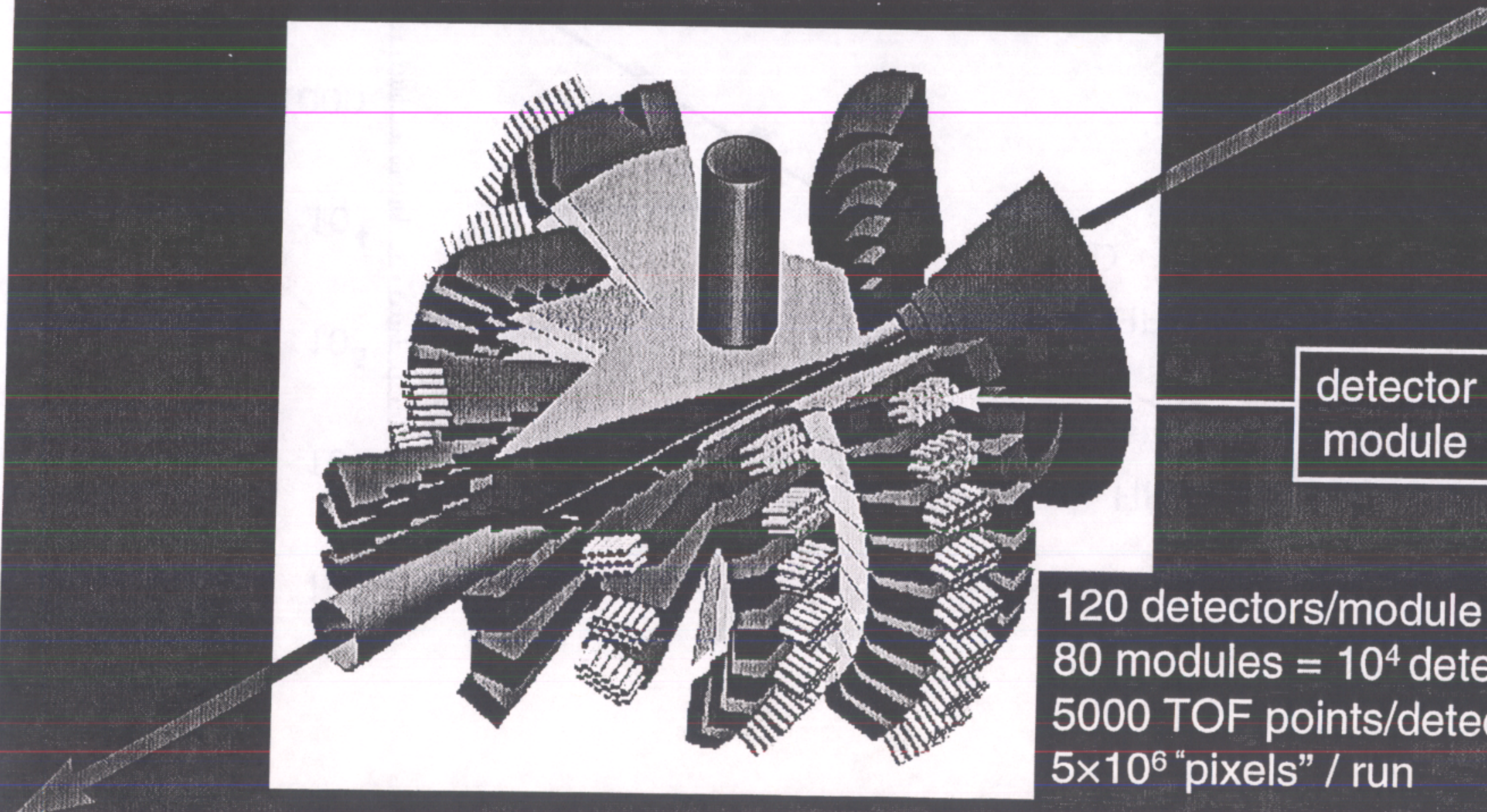
Year	Instrument	Run-time	Data points	Points/day
1983	SEPD	4 hours	3×3000	5.4×10^4
1983	D1b	10 min	400	5.8×10^4
1987	HRPD	2 hours	10000	1.2×10^5
1989	D2b	1 hour	6400	1.5×10^5
1995	POLARIS	20 min	3×3000	6.5×10^5
1997	HRPD	5 min	5000	1.4×10^6
1997	D20	1 min	1600	2.3×10^6



D20
HRPD
Polaris
D2b
D1b
HRPD
D1a(10)
SEPD
Datapoints / day
10^7
10^6
10^5
10^4
1000
100
1960
1980
2000
Year

Data rates (continued)

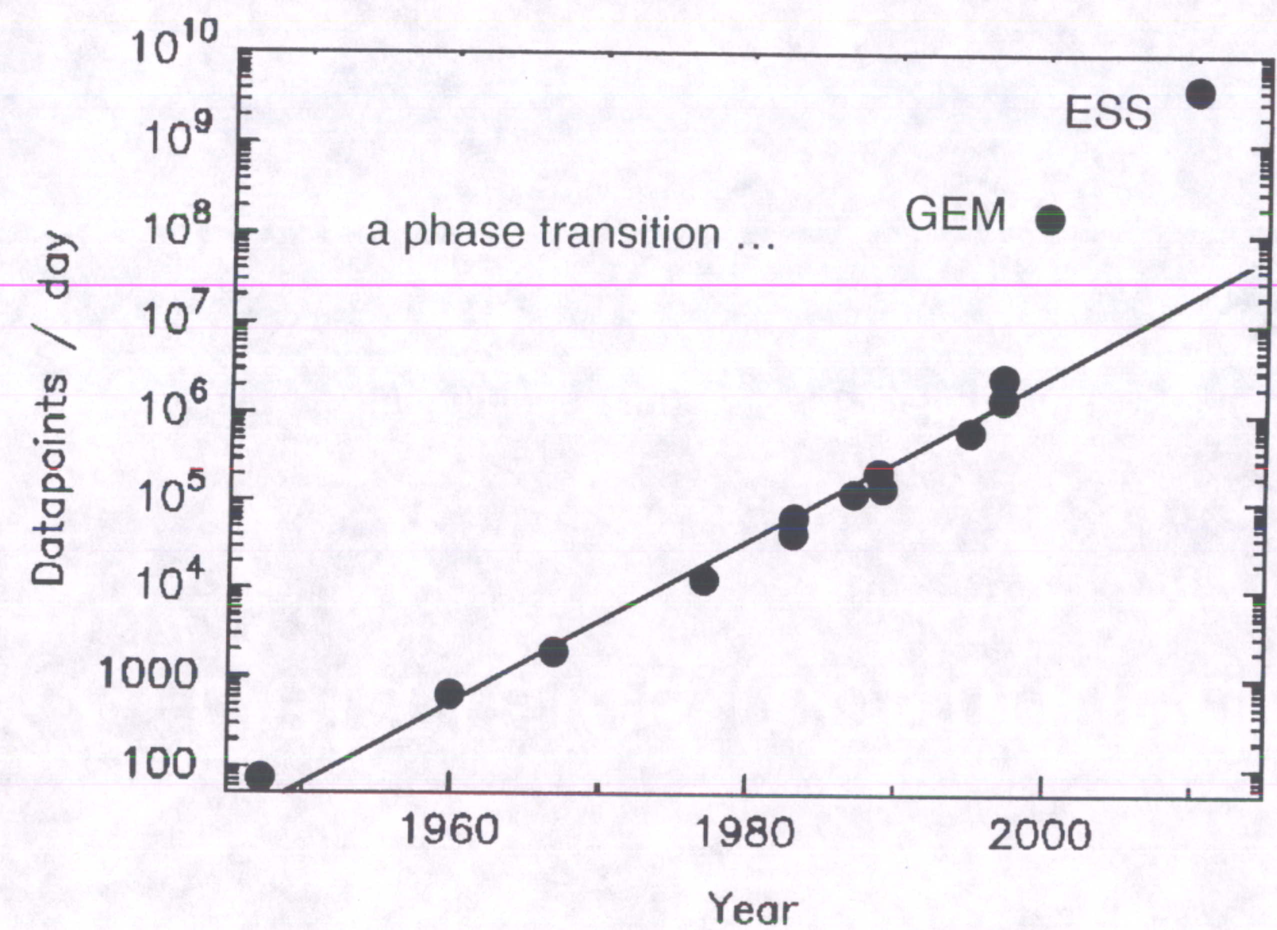
GEM (ISIS) 1999-



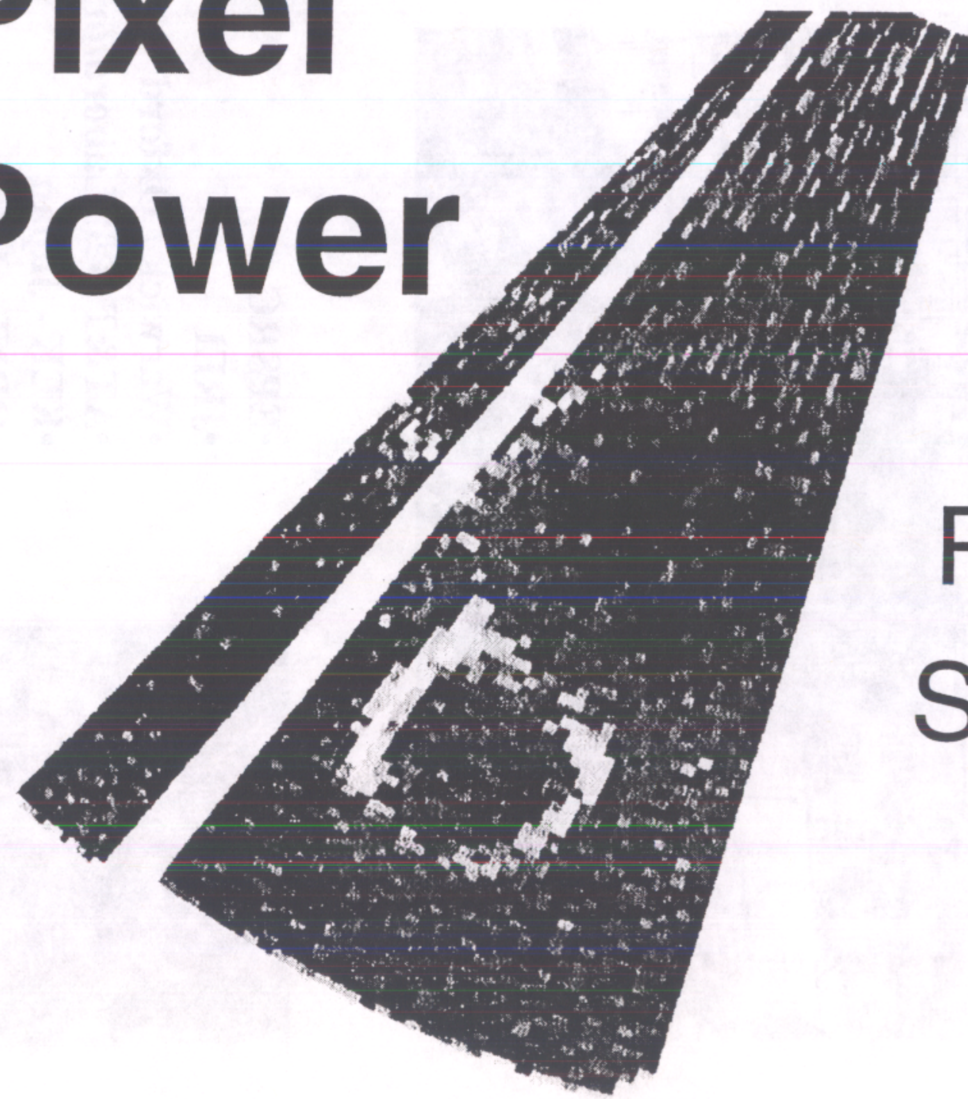
120 detectors/module
80 modules = 10^4 detectors
5000 TOF points/detector
5×10^6 "pixels" / run

Data rates (continued)

Year	Instrument	Run-time	Data points	Points/day
2000	GEM	2 min	5×4000	1.5×10^{8}
2010	GEM(ESS)	4 sec	5×4000	4.5×10^{9}


ESS
GEM
a phase transition ...
Datapoints / day
10^10
10^9
10^8
10^7
10^6
10^5
10^4
1000
100
1960
1980
2000
Year

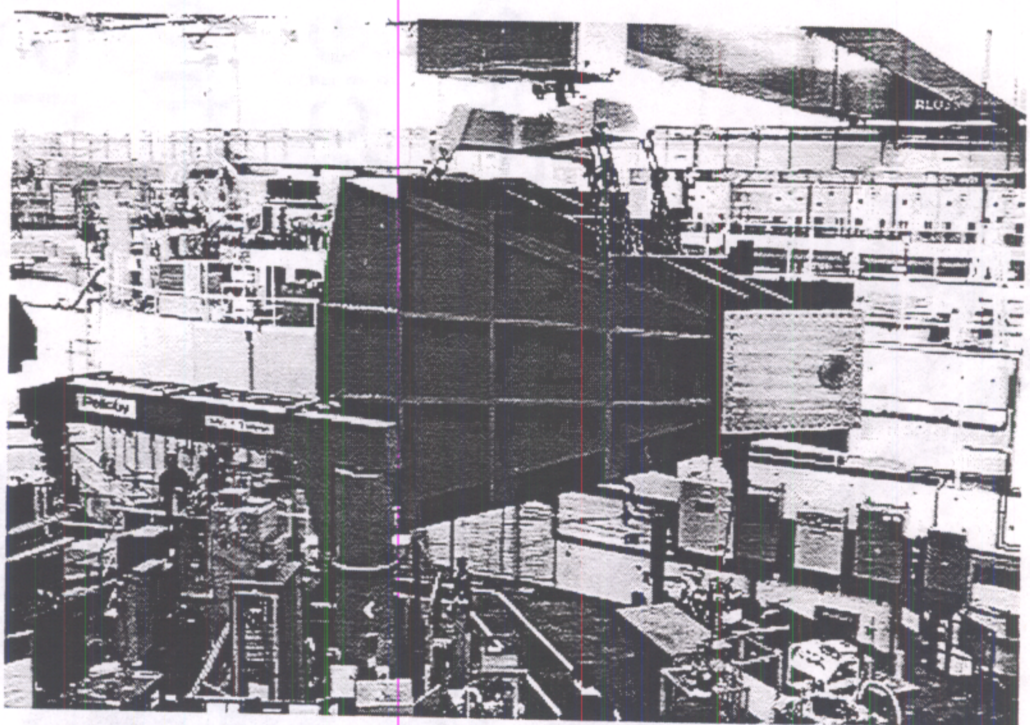
Pixel Power

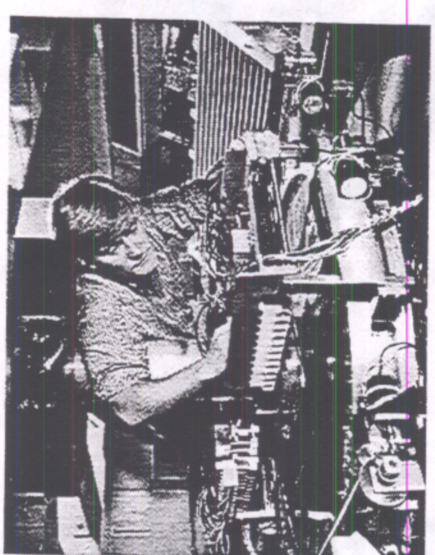


Recent Science from ISIS

ISIS

MAPS - a £3.5M Investment in ISIS

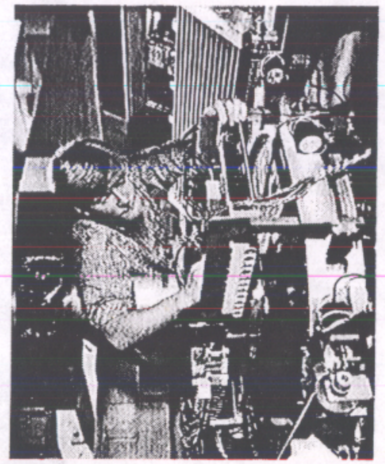


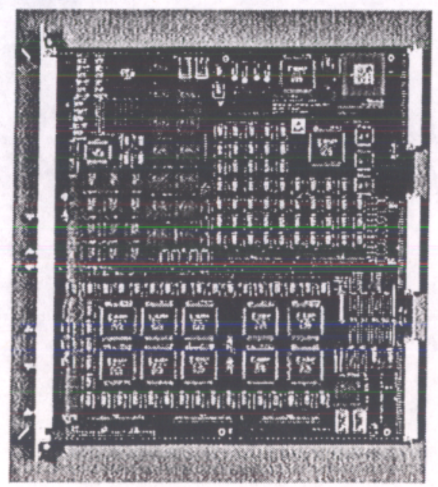


- EPSRC
- JREI
- Warwick / Oxford
- AT&T Bell Laboratories
- KEK - Japan
- ORNL - USA

ISIS

ISIS and Technology Departments - working together





ISIS* - *Science & Engineering Skills
to specify the design

Technology* - *Detector and DAE Skills
to realise the design

HET Prototype	MAPS
1 m^2 detector -	16 m^2 detector -
16 Mbytes	0.5 GBytes

World's Brightest Neutron Source

+

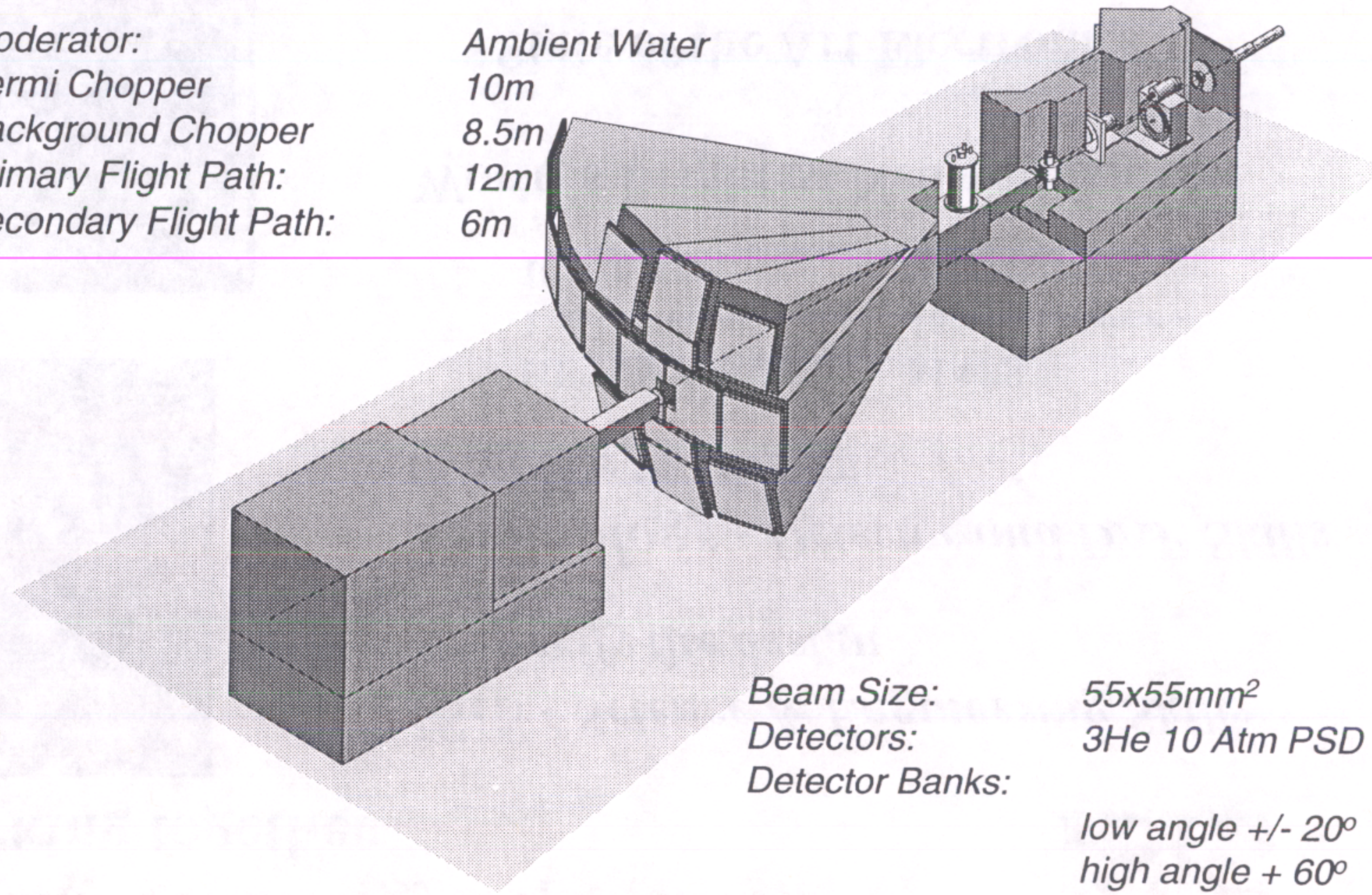
State of the Art Electronics

=

*****PIXEL POWER*****

The Future - MAPS

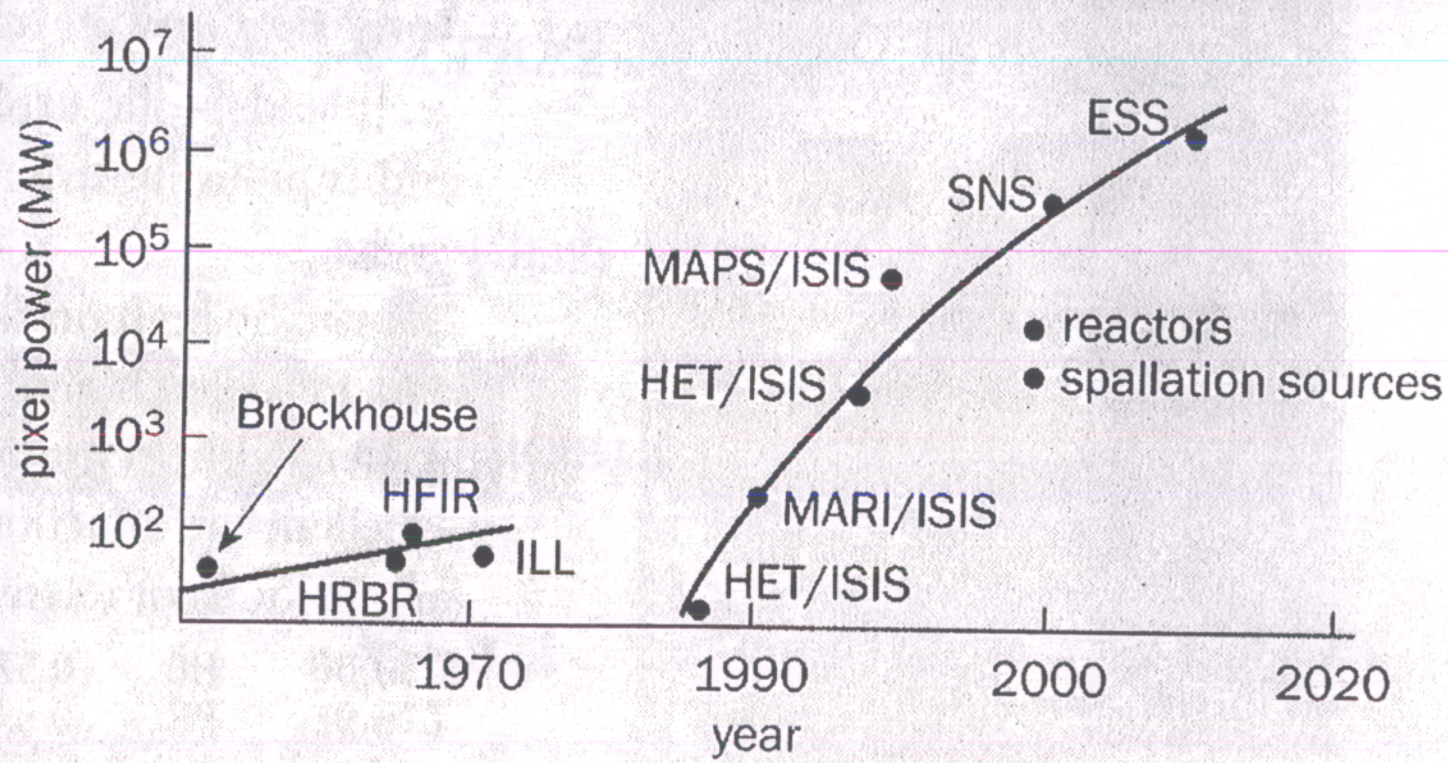
Moderator:	*Ambient Water*
Fermi Chopper	*10m*
Background Chopper	*8.5m*
Primary Flight Path:	*12m*
Secondary Flight Path:	*6m*



Beam Size:	*55x55mm^2*
Detectors:	*3He 10 Atm PSD*
Detector Banks:	*low angle +/- 20°* *high angle + 60°*
Resolution:	*$\Delta\varepsilon/\Delta E_i$ of 2% at elastic position*

ISIS

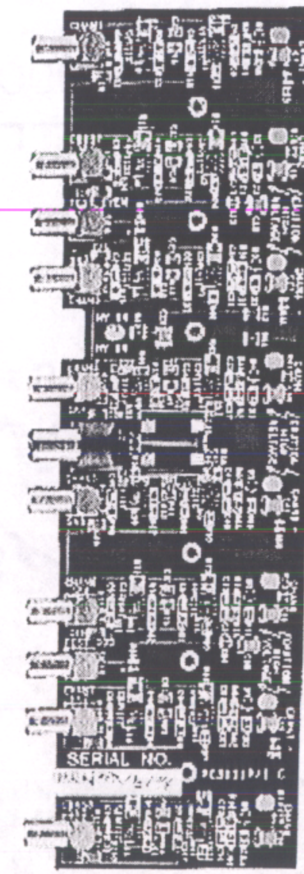
6 IT drives neutron scattering



An approximate measure of the information content obtained from neutron-scattering experiments is the pixel power. New instruments at spallation sources look set to increase the pixel power dramatically.

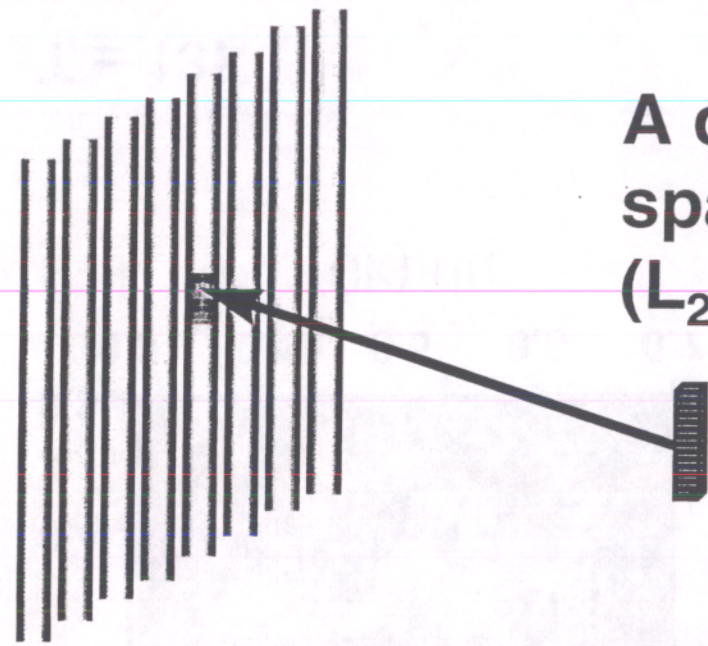
PSDs installed on HET in May '97

- Fast
- Efficient
- Stable
- Good Resolution



ISIS

How to Use the PSDs on HET?



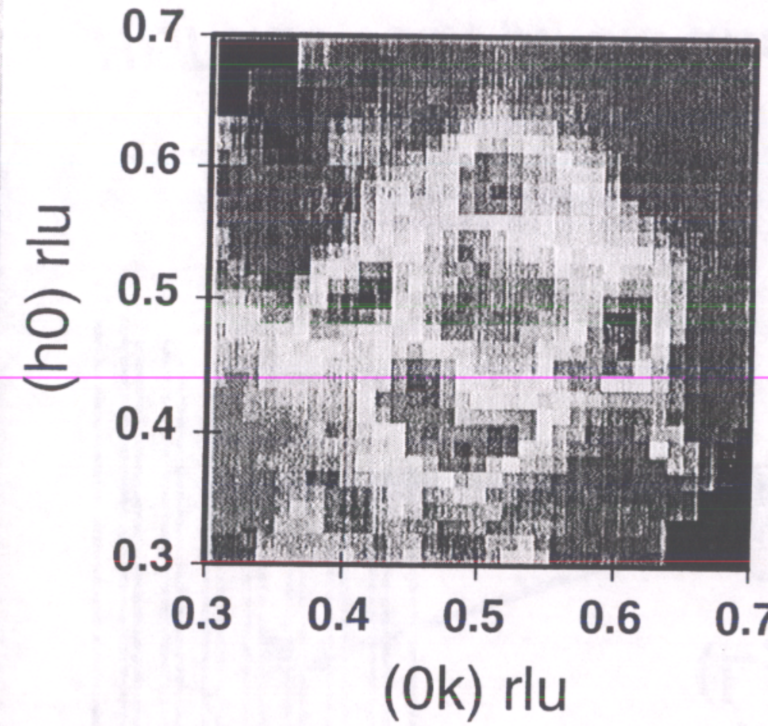
A detector pixel at real space position $(L_2, \theta, \phi, E_t) = (x, y, z, E_t)$

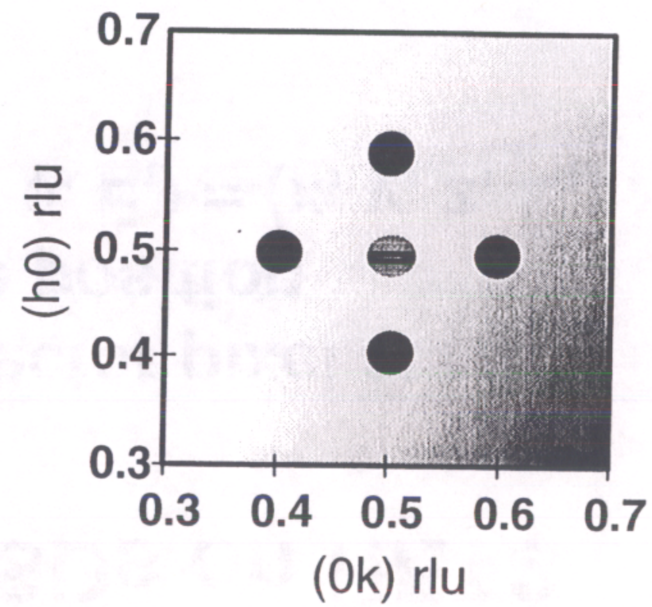
is mapped to a point in reciprocal space at (Q_x, Q_y, Q_z, E_t)

HET has 1664 pixels and typically 100 Energy Bins $=10^5$ points in reciprocal space

ISIS

$YBa_2Cu_3O_{6.6}$





T = 13K

Energy Transfer = 24.5meV

ISIS

Future Developments

X-Rays

Next Generation X-ray Sources are now a reality in Europe, USA + Japan
(6 GeV 7 GeV 8GeV)

Domestic 3rd Generation SR sources (2-3 GeV) being developed in

France	SOLEIL
Switzerland	SLS
UK	DIAMOND

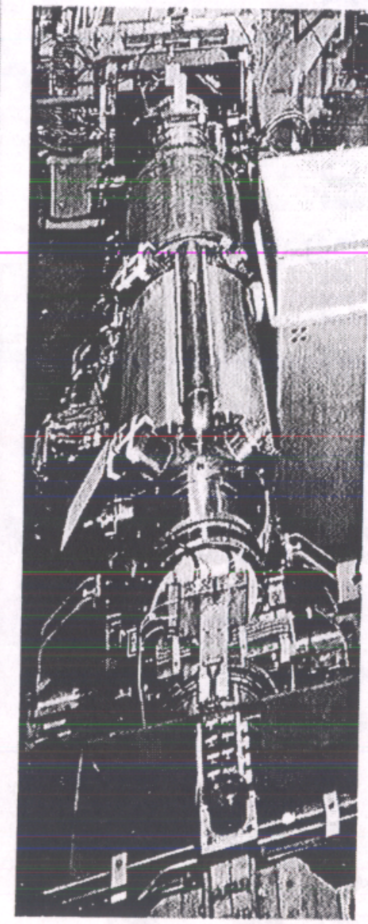
Neutrons

USA and Japan striving to attain ISIS-like capabilities

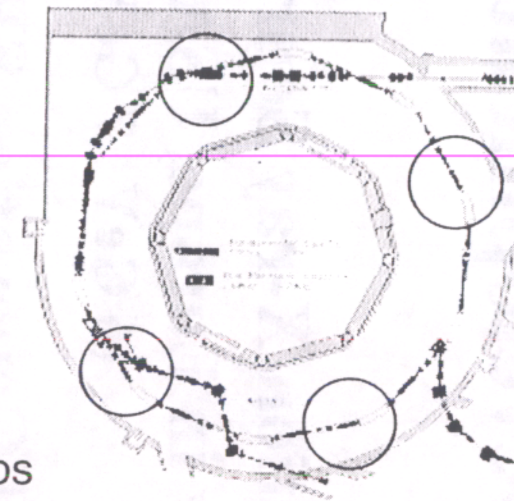
ISIS Upgrades

- 300 uA
- Target II
- SIRIUS

Future Developments
Upgrade to **300 μAmps**



Dual harmonic acceleration in the ISIS synchrotron could upgrade performance to $3.7x10^{13}$ protons per pulse



- Beam current of 300 μAmps
- No loss of beam current if a 2nd Target station is installed
- Radioactive nuclear beam research - SIRIUS

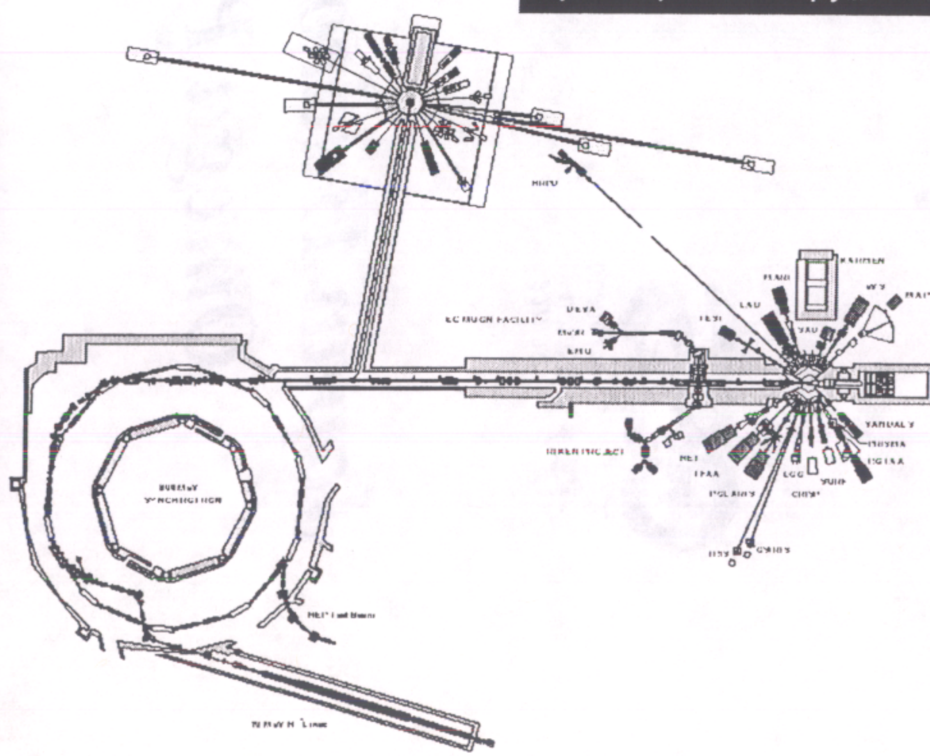
ISIS

Future Developments

A Second Target Station

A second, low frequency, target station optimised for

- Reflectometry
- Small Angle Scattering
- Neutron Spin Echo
- High Resolution Diffraction
- µeV Spectroscopy



Soft Condensed Matter
polymers
colloids
surfactants

Biotechnology
drug molecules
small proteins
food science

Complex Structures
zeolites
clathrates

Surfaces and Interfaces
spin valves
magnetic thin films
LB films
electrochemistry

ISIS

Next Generation Neutron Sources

Developments beyond ISIS

ess european spallation source

SNS

Japan Hadron Facility Omega Project

Increased Source Strength

1930s & 1940s
- Total cross-sections

nuclear physics

1950s
- Structural Studies

crystallography

1960s
- Dynamical Studies

physics

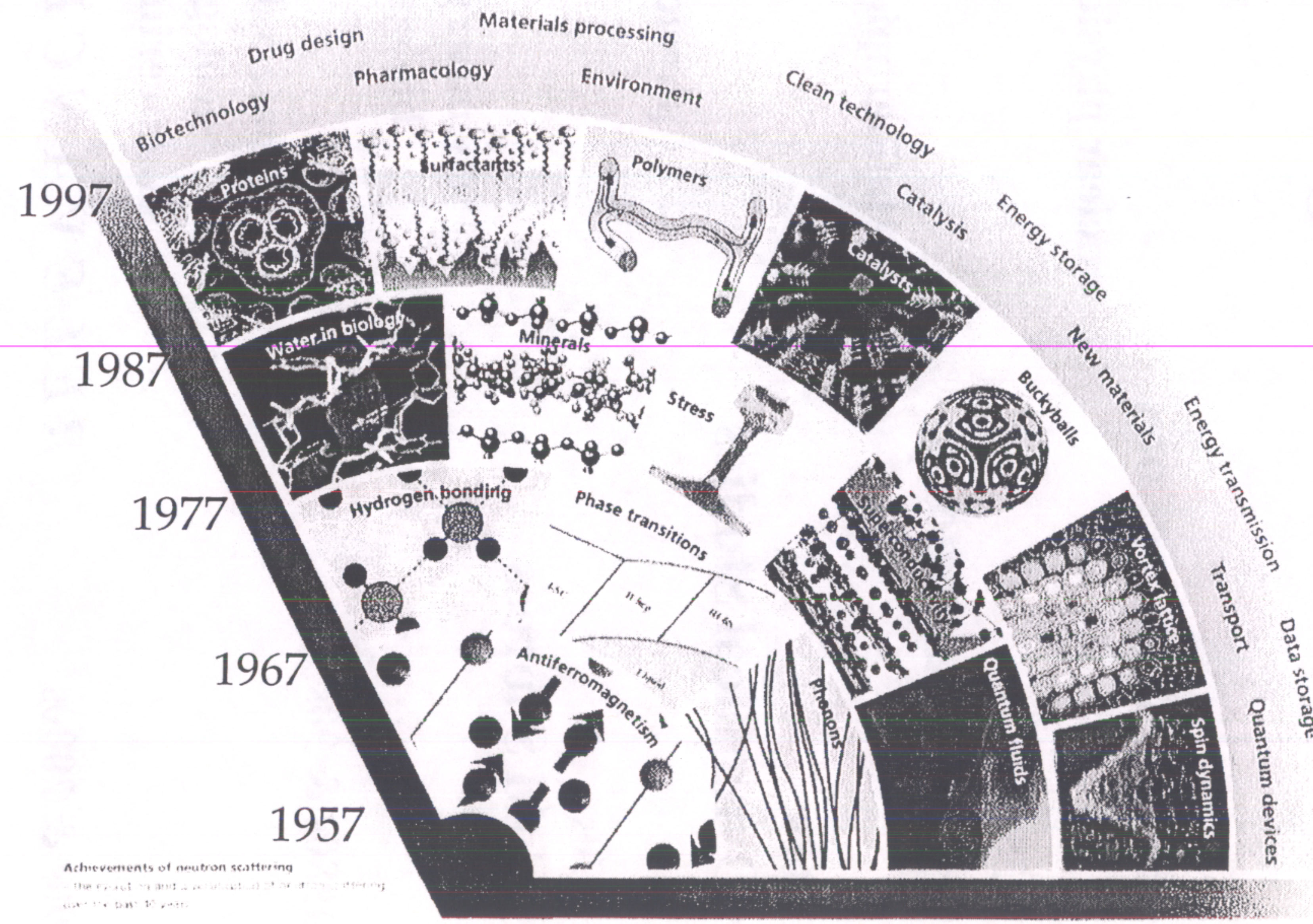
1970s
- Cold Sources

chemistry
biology

1980s & 90s

materials
geology
engineering

90s & 2000s — *R E L E V A N C E*



Achievements of neutron scattering

Need for a Next Generation European Neutron Source

Neutron Scattering is Intensity Limited

Better Resolution

- True from astronomy to microscopy

Smaller Systems

- crack tip
- dilute solutions
- new materials

Shorter Experiments

- kinetics
- extreme environments

Complex System

- wide Q, ω range
- good resolution
- high signal-to-noise

Advanced Techniques

- polarisation analysis

Need for a Next Generation European Neutron Source

An example

High Temperature Superconductors

Structure

Possible on powder samples

Dynamics

Requires large single crystals

- phonons
- exchange interaction

Parametric studies

T, x, P, H....

Illustrations of Need for a Next Generation Neutron Source
(Slides not included)

Structure **of YBCO first correctly determined at ISIS in 1987 (Front Cover of Nature)**

Dynamics **required a massive 0.1 kg crystal which took until 1991 (PRL). With such a crystal fundamental information on the interaction strengths could be determined in a 4 week experiment: parametric studies - although feasible are impractical because of source strength**

Kinetic studies **of the solid state chemical reactions *in situ* in a Duracell battery during discharge leading to a microscopic understanding of why the battery holds only half the theoretical charge**

Uses of a Next Generation Neutron Source

Real Time Experiments
in situ studies

Alchemy

⇩

⇩

Understanding

Metastable compounds

- new battery materials
- high Tc systems

Chemical Processes

- catalytic loading
- battery discharge

European Science Foundation Study: Conclusions

- The use of neutrons continues to evolve, both in traditional and in new fields. Given the enormous impact of new materials in technology, no end to this process can be foreseen. The demand for more sophisticated use of neutrons continues to grow, so that aggressive programmes of instrumentation development are vital to the field.
- Non-neutron tools for matter investigation, such as synchrotron radiation, cannot substitute for the future use of neutron beams.
- The diversification of neutrons into a number of wider scientific areas continues. Examples are earth sciences, pharmaceutical sciences, biology and engineering.
- The direct impact of neutrons on 'wealth creation' is increasing and will continue to do so. Examples of industrial relevance are in the fields of multilayers, polymers, materials science, and engineering.
- Unless appropriate action is taken, sources of neutrons, and hence the supply, are likely to *decrease* in the next ten years.
- Given the existing and future expected demand in Europe this makes it imperative that:

  (a) full use be made by European users from the basic and applied sciences of the present network of medium-flux national sources and the highest flux sources - ILL and ISIS, and

  (b) a mechanism be initiated by the ESF to co-ordinate the design and funding requests that will allow a truly advanced European Source to be operational within 15 years.

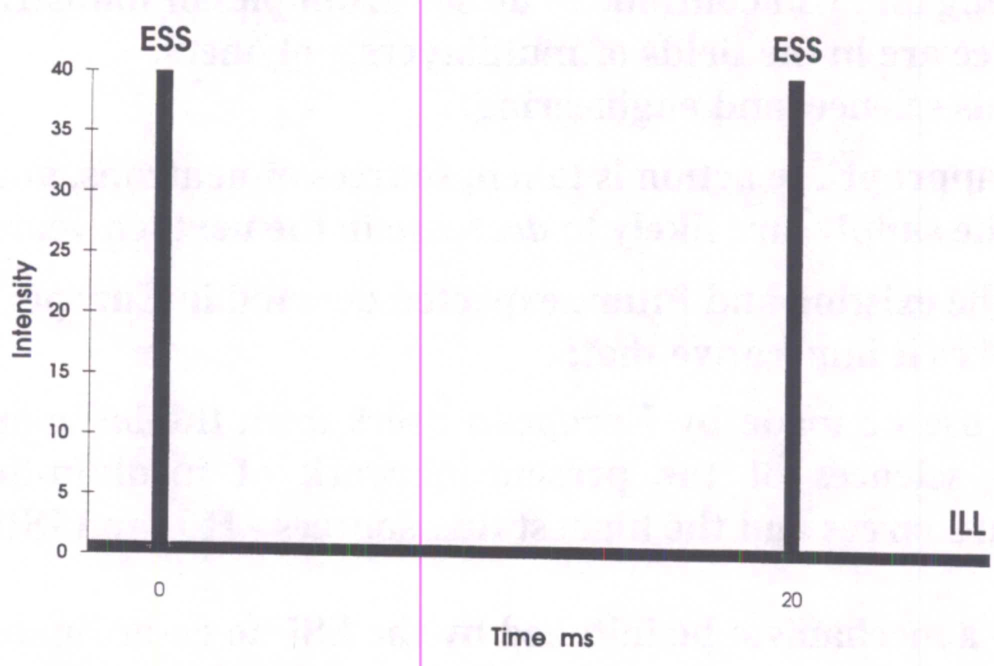
European Spallation Source

Specification

- 5 MW
- ~ 1 μs pulse
- 50Hz and 10Hz Targets

Performance

- 30 x ISIS
- Φ equivalent to ILL but *PULSED*
  qualitatively different source



European Involvement in ESS Science Case

200 Scientists from 15 European Countries

Austria, Czech Republic, Denmark, France, Germany, Italy, Netherlands, Poland, Portugal, Russia, Slovenia, Spain, Sweden, Switzerland, UK

European Involvement in ESS Technical Study

100 Scientists and Engineers from 20 Institutes

Memorandum of Understanding
for
ESS R&D Phase
signed on
5 May 1997
between

Denmark, France, Germany, Switzerland & UK

Spain (*CIEMAT*), Netherlands (*IRI*), Italy (*INFM*), Germany (*HMI*) & Germany (*JWGU*)

19 May 1998

ESS Layouts timescales and costings from ESS Volume I

(Not included)

ESS R&D Phase

1998 -2000 (2002 ?)

- *Site independent study*
- *Reduce technical risks*
- *Minimise costs*
- *Database for the engineering design*
- *Safety and Licensing issues*
- *Timetable and budget profile*
- *Proposal for instrumentation*

Accelerator - Gardner (RAL)
Targets/Engineering - Bauer (PSI)/Ullmaier(Julich)
Instrumentation - Steiner (HMI)

OECD Megascience Forum

Neutron Sources WG

Three tier strategy:

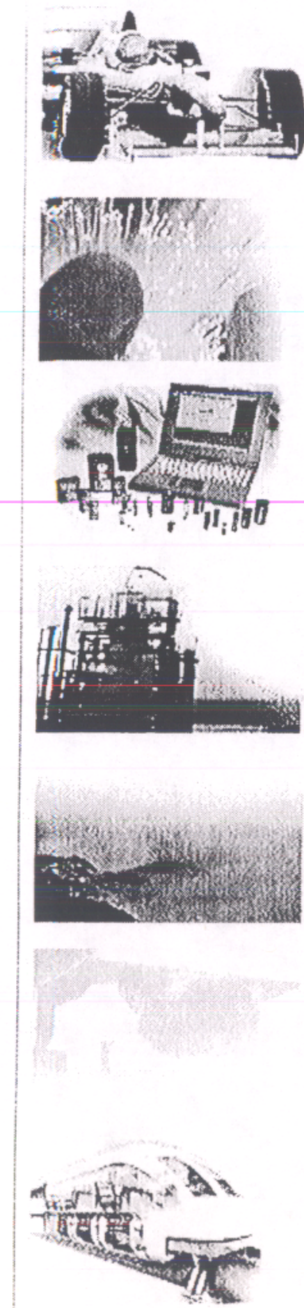
- to maintain, as far as appropriate, existing national sources
- to maximise the utilisation and potential of current front rank facilities
- to prepare for the provision of next-generation regional sources

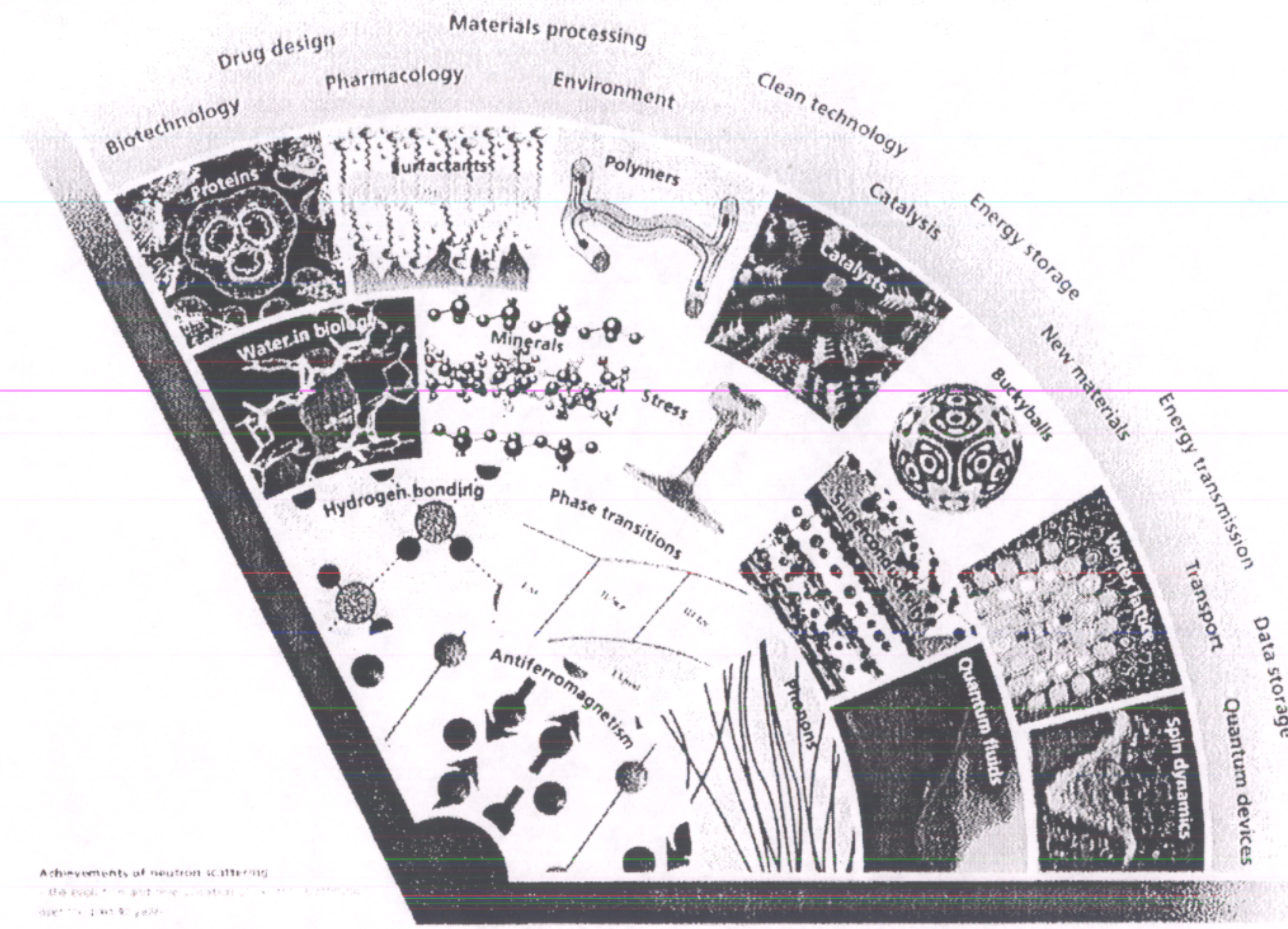
Detectors are Key

@ heart of the problem

- *Greater Efficiency*
- *Higher Data Rates*
- *Smaller Pixel Size*

- *Lower costs*





Achievements of neutron scattering

The future for neutrons is bright.