ISIS-II: Science Capabilities

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ISIS-II Webinar

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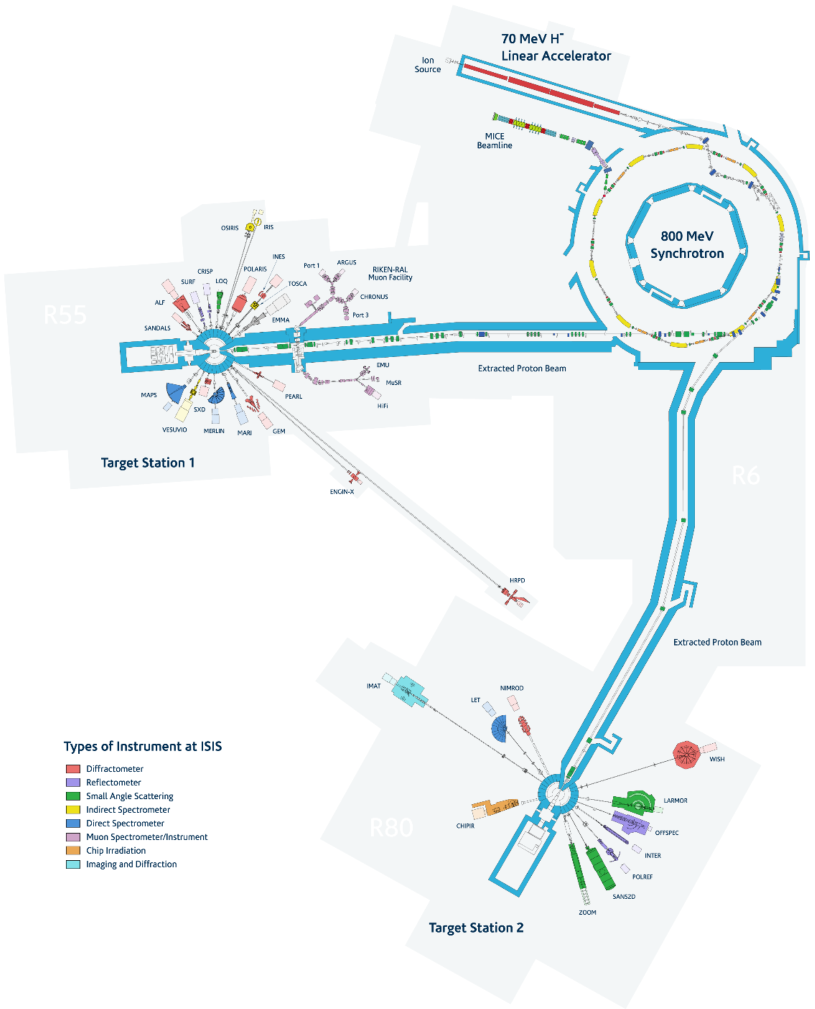
Science and Technology Facilities Council
ISIS Neutron and Muon Source

Outline

- **Brief Introduction to ISIS Science Directorate**
  - *What we do*
  - *Science Strategy*
- **Science Case for ISIS-II**
  - *Parameters Task – Science*
  - *Gain Factors*
- **Summary**



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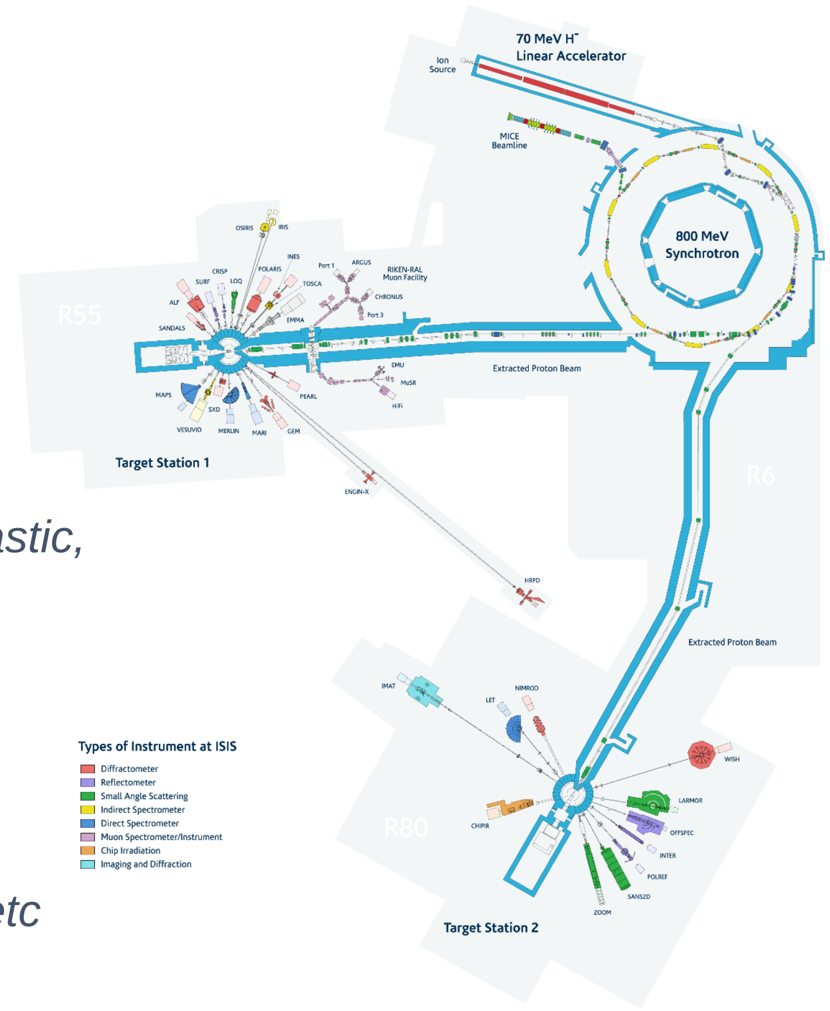
What we do now

- **Structure (and morphology)**
  - *Powder diffractometers*
  - *Liquid diffractometers*
  - *Small-angle scattering*
  - *Neutron reflectometers*
  - *Imaging/tomography*
- **Dynamics**
  - *Neutron spectrometers (inelastic and quasi-elastic, Larmor procession*
  - *Muon spectrometers*
- **Others**
  - *Irradiation facility*
  - *Support labs*
  - *Computing – ISIS based, SCD, Hartree, ALC etc*
  - *Test facilities*



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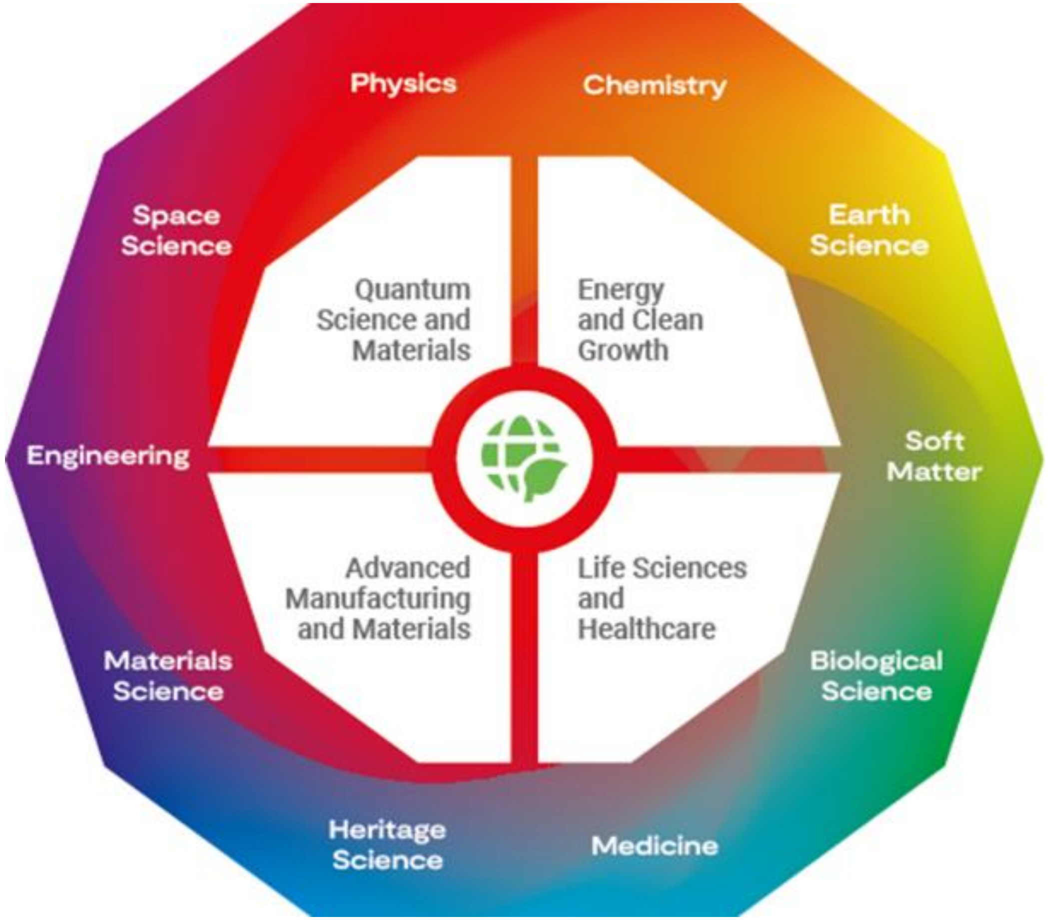
ISIS Science Strategy

- Maximise our impact on important scientific, economic and societal challenges through focus, leadership and collaboration with academic and industry partners
- Translate our fundamental insight of matter to applications
- Support, collaborate and grow our academic and industrial communities
- Motivate the next generation of technicians, engineers and scientists

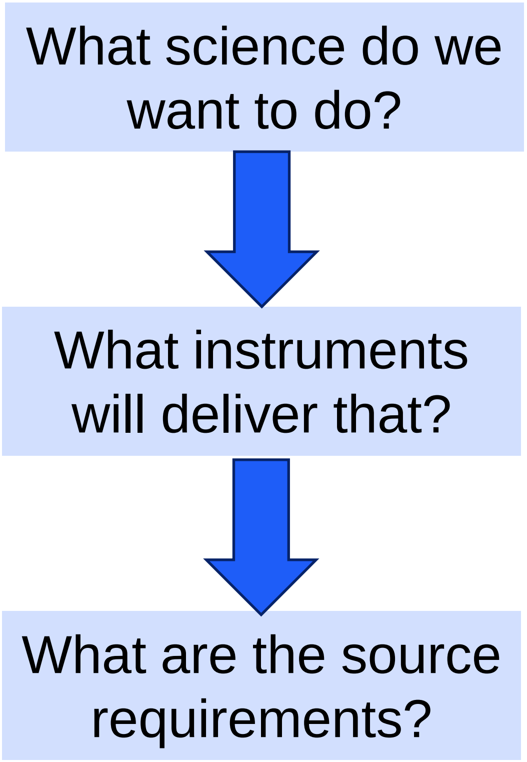


Science Case for ISIS-II

What have we done so far…

Parameters Task

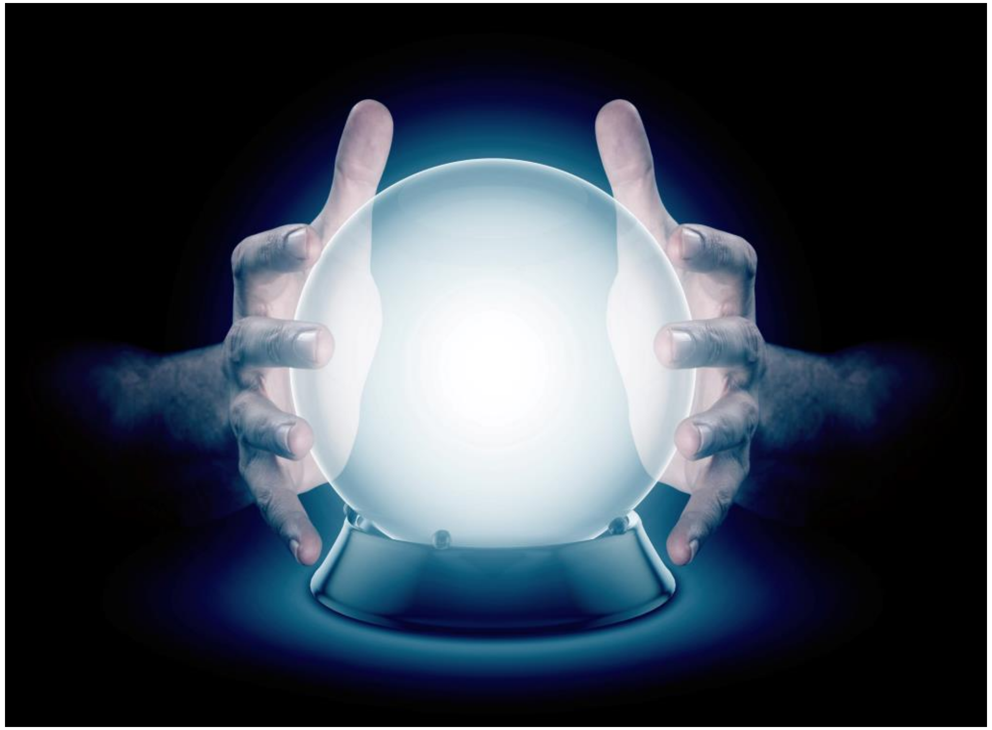
- First attempt to prepare a science case and explore instrument and source requirements
- Science GLs (and a few others!) presented the Science Group views
- Complemented by talks on instrumentation and source components including accelerator, moderators, target, reflector and electrical supply
- Other facilities



What science will we be doing in 10 – 20 years?

Numerous factors to consider

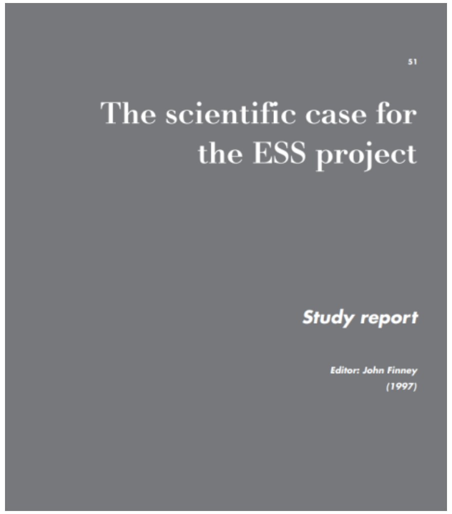
- Government research priorities
- Other sources – old and new
- Other techniques – complementary and competitive
- View of the scientific community
  - *Current ISIS Users*
  - *Current other facility users*
  - *Researchers who don't use the facilities (but could benefit!)*



What science will we be doing in 10 – 20 years?

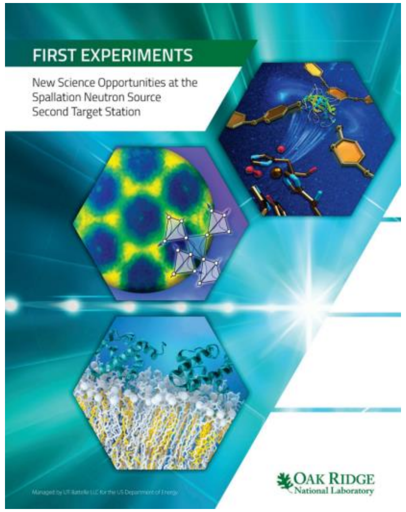
What we do now

- ISIS science programme is very broad
  - *Physics*
  - *Chemistry*
  - *Materials Science*
  - *Biology*
  - *Engineering*
  - *Earth Science*
  - *Planetary Science*
  - *Cultural Heritage…*
- These are what neutrons and muons excel in
- Likely the areas will stay the same
- Increasingly researchers use more than one technique



The scientific impact of ESS in specific areas

Polymers and soft matter
Disordered materials
Structural materials chemistry
Chemical reactivity and molecular motions
Biology and biotechnology
Earth and environmental science
Engineering
Condensed matter and materials physics
Fundamental neutron physics
Exploitation of other particle sources at ESS



First experiments. SNS Second Target Station

Polymers and soft materials
Quantum matter
Materials synthesis
Energy materials
Structural materials
Biology and life sciences

Science driven source parameters

What Science do we want to do

What Instruments will deliver this science

What requirements does the place on the source

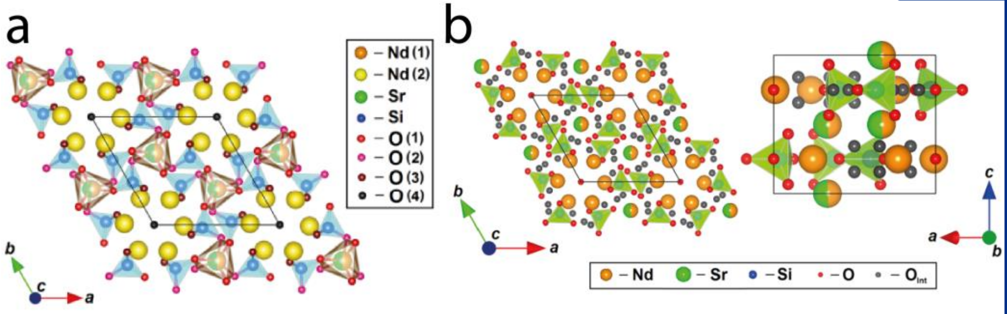


Figure 2.1.5. a) neutron-determined crystal structure of $Nd_8Sr_2Si_6O_{26}$ and **b)** distinction between the static (red spheres) and interstitial (grey spheres) oxygen sites. Figure is adapted from the original manuscript.

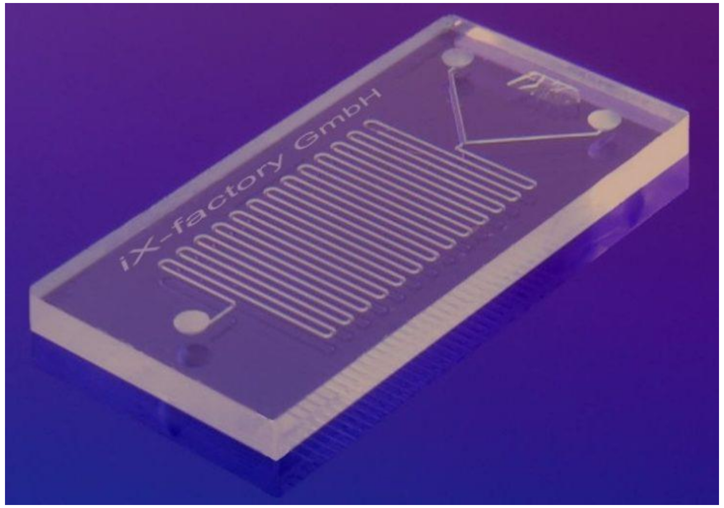
Very broad range of applications

Enhanced In-situ/ in-operando

Requirements for multiple instruments and high throughput

Smaller samples

- Reduce by an order of magnitude
- New frontiers for diffraction and spectroscopy
- Open up in-operando studies
- Engineering gauge volume
- Highly absorbing materials
- External variables (H, P, T)



Science driven source parameters

What Science do we want to do → What Instruments will deliver this science → What requirements does the place on the source

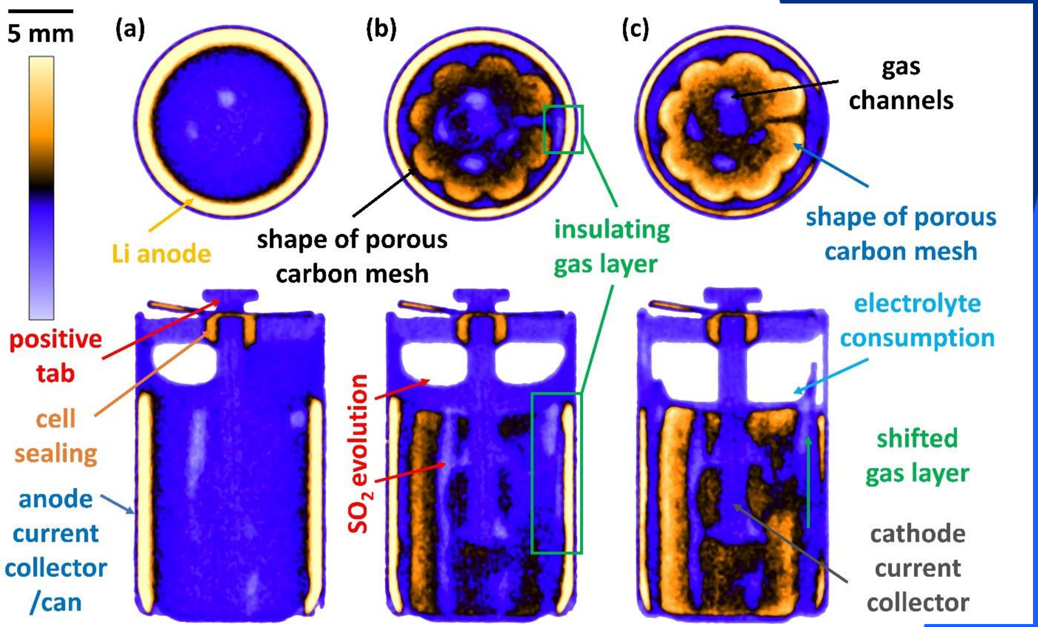
Very broad range of applications

Enhanced In-situ/ in-operando

Requirements for multiple instruments and high throughput

Faster measurements

- Reduce counting time an order of magnitude
- Kinetics
- Complex energy materials
- Fast Rietveld



R. Ziesche

Science driven source parameters

What Science do we want to do → What Instruments will deliver this science → What requirements does the place on the source

Very broad range of applications

Enhanced In-situ/ in-operando

Requirements for multiple instruments and high throughput

Enhanced complexity

- Disordered materials
- Multiphase
- Multi-modal
- Low background measurements

Technological relevance

Support infrastructure

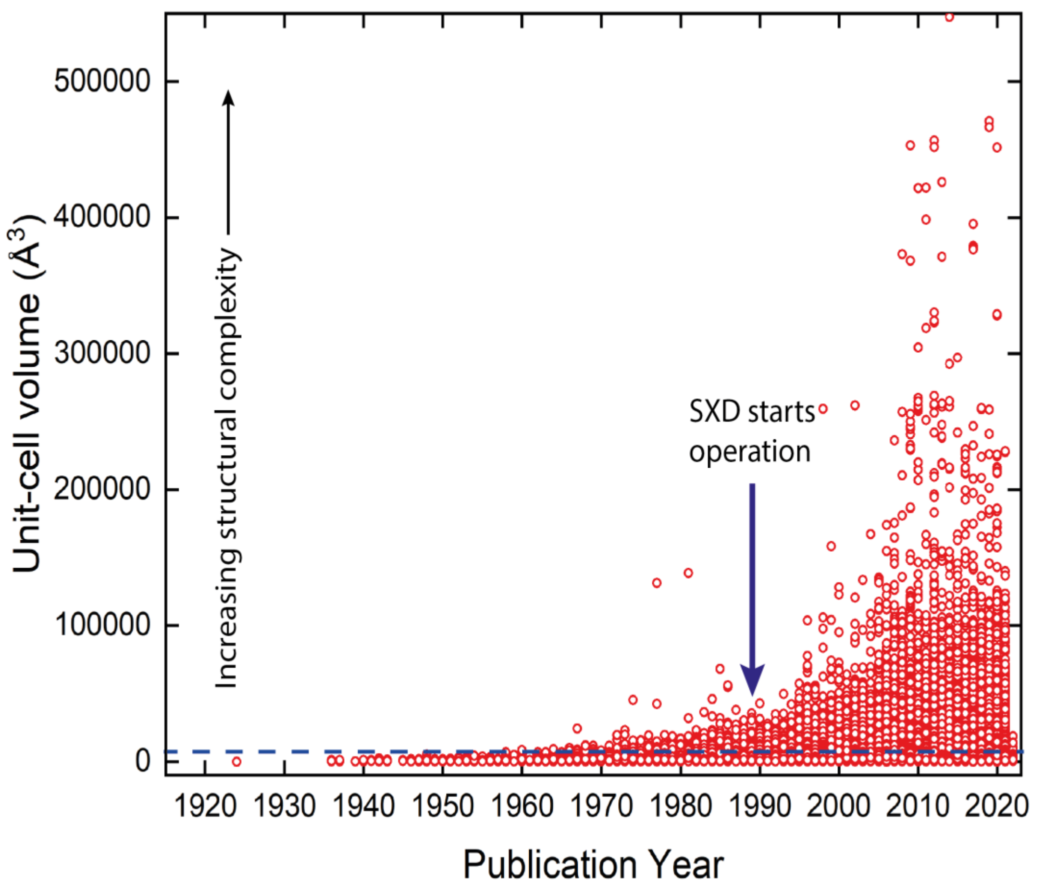


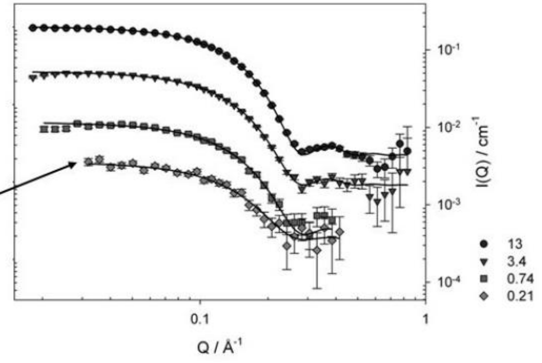
Figure 2.1. Unit cell volume versus publication year of crystal structures in the CSD. The blue dashed line indicates the upper limit of the unit cell volume that can currently be measured on SXD.

Science driven source parameters

What Science do we want to do

What Instruments will deliver this science

What requirements does the place on the source



More long wavelength neutrons needed!

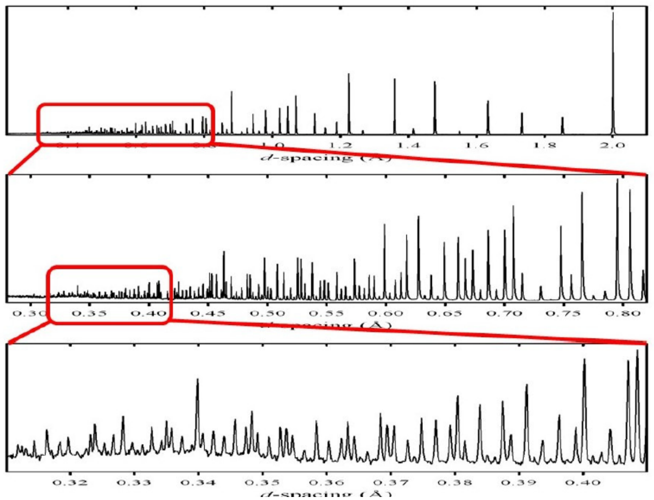
Very broad range of applications

Enhanced In-situ/ in-operando

Requirements for multiple instruments and high throughput

To achieve the science parameters

- Higher flux
- Wider energy range
- Higher resolution
- Lower backgrounds
- Source reliability



Requirements matrix – not one solution for all!

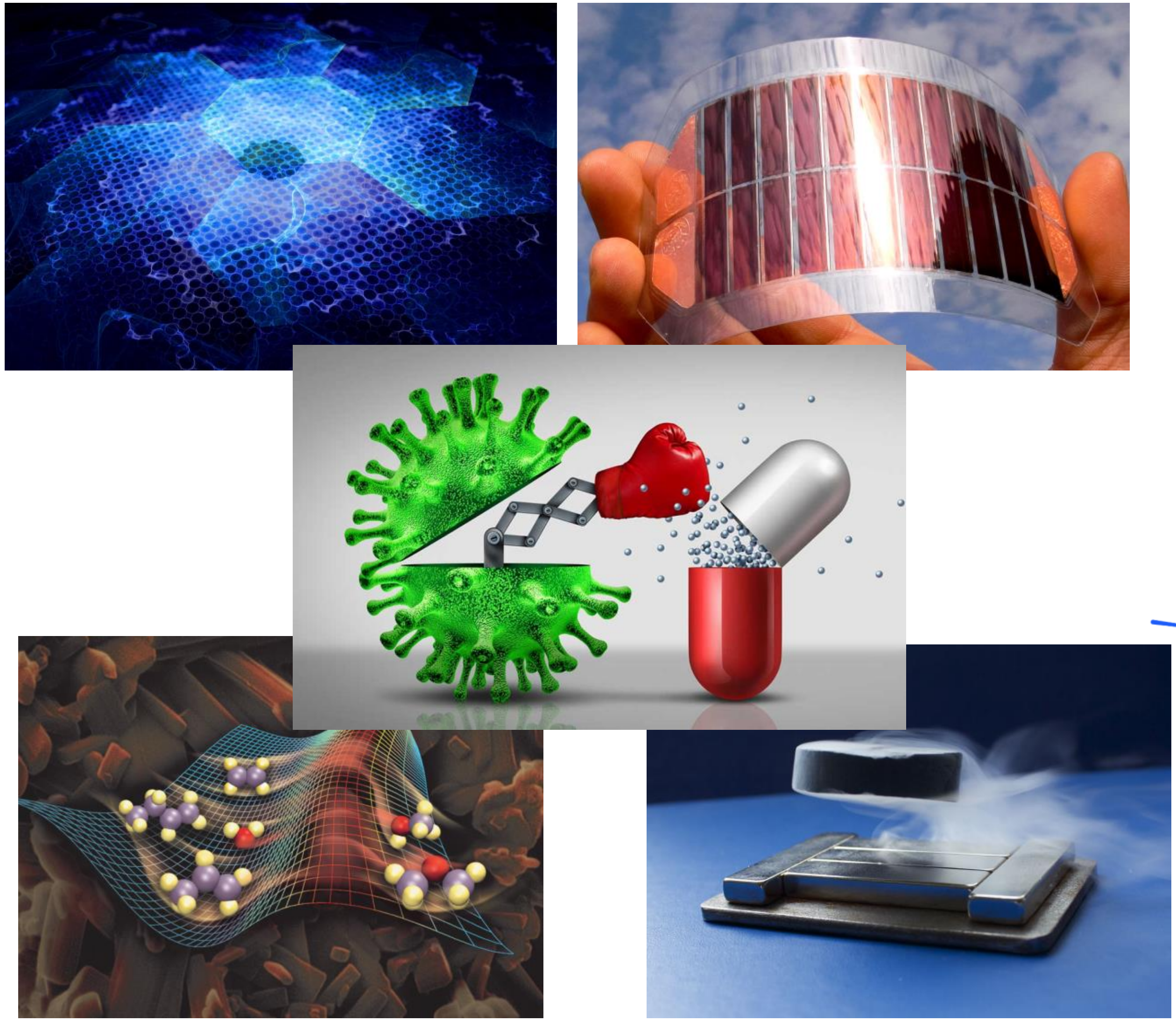
Gain factors

This has let do a Gains Report being written to look to answer

- *How small?*
- *How fast?*
- *How complex?*

For each of the Science Groups

Thanks to Steve Lilley



Gain factors

What is facility gain?

Improvement in a metric over a baseline

Here ISIS post Endeavour is the baseline

Facility is broken down into source and instrument

Assumed that the instrument gain is independent of the source gain

Different for different techniques

Muons and Irradiation have a different set of metrics still!

Technique	Low gain (<5)	Medium gain (5-10)	High Gain (10-25)	Very High Gain (25+)
Excitations				
Crystallography				
Molecular Spectrometry				
Reflectometry				
SANS				
Disordered Materials				
Engineering and Imaging				

Outcome	colour
Unable to benefit from	
Capacity Increase	
Transformative capability	
Limited capability, mostly capacity	

Summary of the Gains Report

Not one facility fits all

Typically, low gains

- *Little to no impact on balance of the programme*
- *Increase in capacity only*

Typically, medium gains

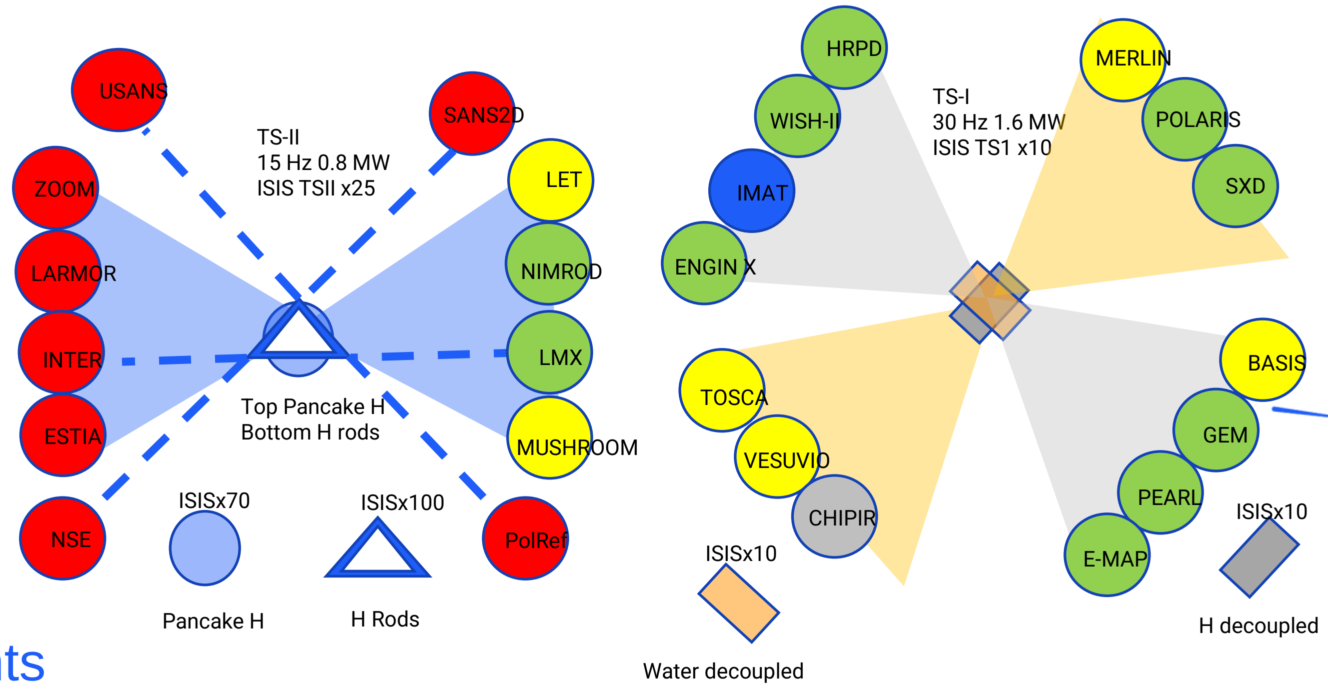
- *Can provide new science*

Large gains will allow

- *New science to be performed*
- *'Real' systems to be studied*

S/N is key for the majority of instruments

Even modest gains require significant increase in supporting infrastructure



Summary

- **The current Science Strategy is well aligned with other facilities**
- **It is unlikely the areas of science studied will change dramatically**
- **There is a drive to**
  - *Use smaller samples*
  - *Take faster measurements*
  - *Carry out more complex experiments*
- **The source will need to balance**
  - *Flux*
  - *Resolution*
  - *Background*
  - *Energy range*
- **There is not one solution**
- **Even small gains require increase in support infrastructure**

Thank you!

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