A monochromatic powder diffraction instrument for the ESS(SD037)

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- diffraction

LPSS and t-o-f diffraction

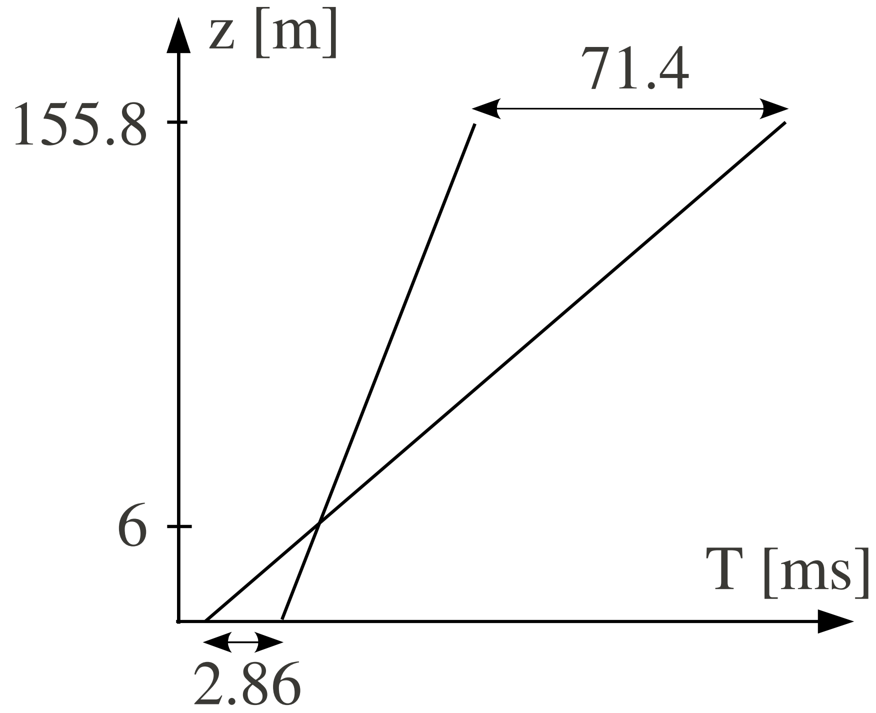
- Diffraction requires low $\Delta\lambda / \lambda$ uncertainty
- Instrument length (moderator – detector) is given by:

$$L = \tau / ((\Delta\lambda / \lambda)\, \alpha\, \lambda_{mean})$$

- For ESS where τ = 2.86 ms, α = 0.2528 ms Å^{-1} m^{-1} and a thermal neutron (λ_{mean} is 1.5 Å)
- 0.1 % resolution requires a 7.5 km instrument
- 0.5 % is 1.5 km
- Even a 'cold' neutron instrument with λ_{mean} of 4 Å and 1 % resolution is 283 m.
- We cannot use the full pulse for any type of diffraction
- A pulse-shaping chopper is needed
- Pulse-shaping brings other limitations

Pulse-shaping chopper

$$\lambda_{max} - \lambda_{min} = \frac{T - \tau}{\alpha L_{det}}$$
$$= \frac{(71.4 - 2.86)\mathrm{ms}}{0.2528\frac{\mathrm{ms}}{\mathrm{\AA m}}155.8\mathrm{m}}$$
$$= 1.74\mathrm{\AA}$$



How much of the long-pulse can be used?

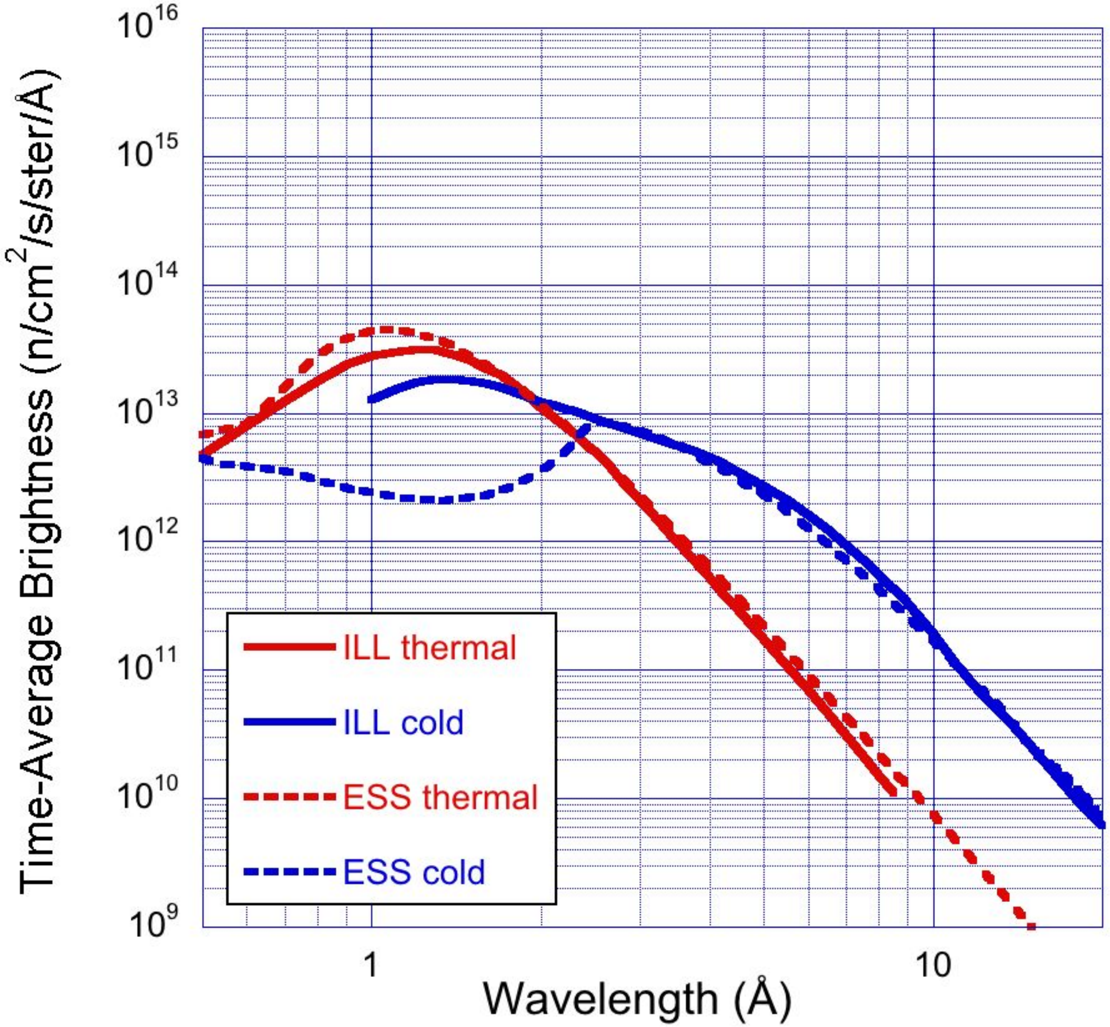
For a 150+6 m instrument:
Δλ/λ 0.1 % useful τ is 57 μs (2 % of full pulse), wavelength band 1.81 Å
Δλ/λ 0.5 % useful τ is 285 μs (10 % of full pulse), wavelength band 1.80 Å

Powder possibilities

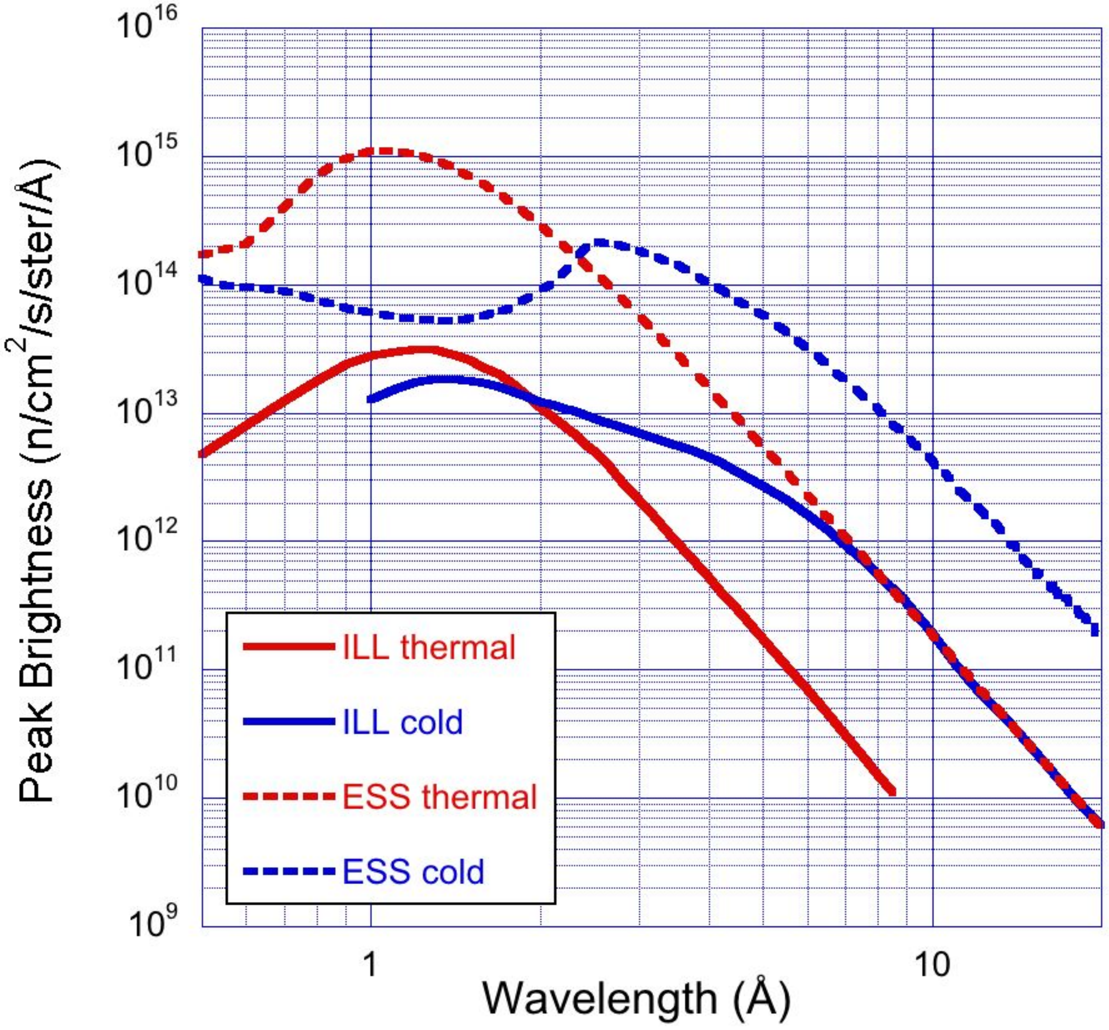
- Wavelength frame multiplication (WFM)
  - Increases available bandwidth
  - Shorter instrument
  - Flexible resolution
  - Flexible choice of bandwidth
  - Uses less of long pulse at constant $\Delta\lambda / \lambda$ cf. natural length instrument
  - No flux gain cf. SPSS instruments, except at larger $\Delta\lambda / \lambda$
  - Mechanical choppers limit Q_{max} (λ_{min})

- Monochromatic
  - Uses full pulse
  - Short(er) instrument
  - Flexible resolution/flux trade
  - Limited choice of incident wavelengths
  - Limited Q_{max}
  - No source gains
  - No gain factor cf. D20

ILL v ESS time average



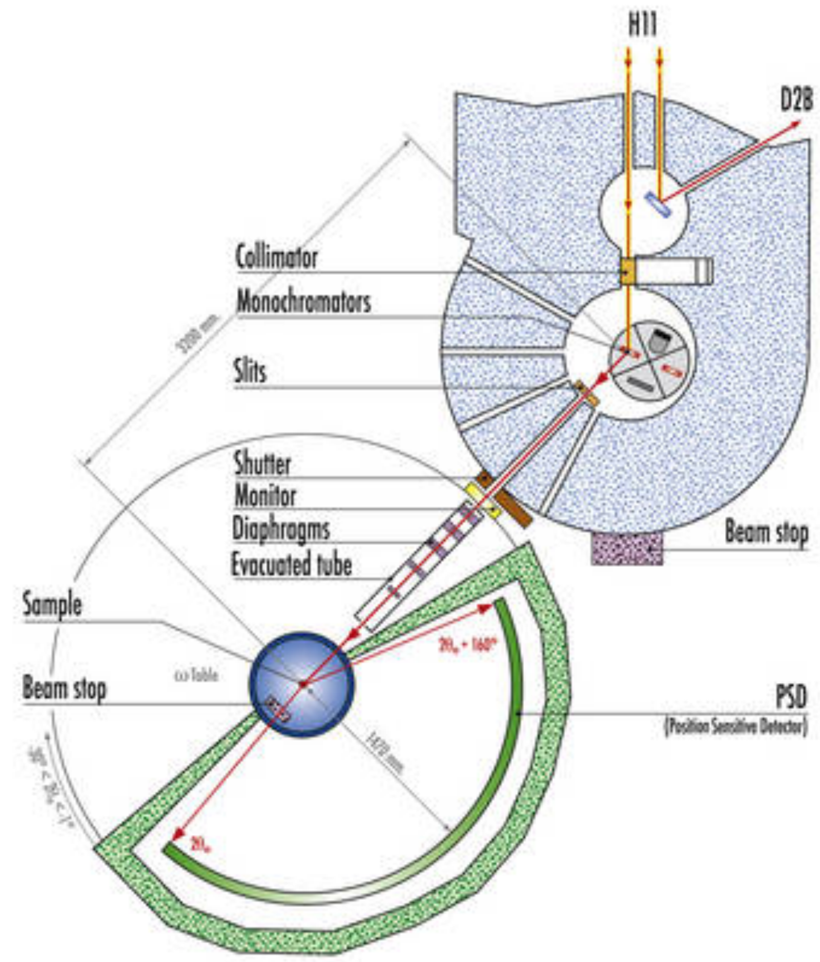
ILL v ESS single pulse



EUROPEAN SPALLATION SOURCE

Concept: Pulsed D20

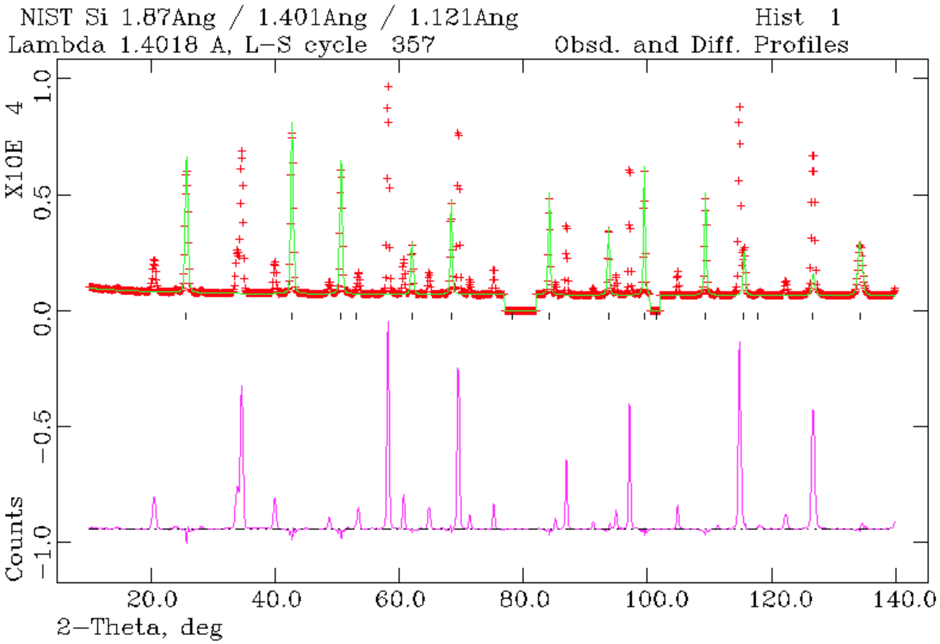
- Primary guide
  - Feeder
  - Half-elliptical guide?
  - Straight v non line of sight guide
  - Possibility of farm (as with H11 at ILL)
- Investigate monochromators
  - Germanium
  - Diamond
  - Composite
  - Others?
- Larger area detector
  - t-o-f resolution
  - Event recording
- Sample environment
  - Optimise for instrument geometry
- New capabilities cf. reactor instrument
  - Multi-wavelength data collection
  - Separate coherent/incoherent scattering
  - Elastic/inelastic/QENS measurements
  - Fast kinetic measurements

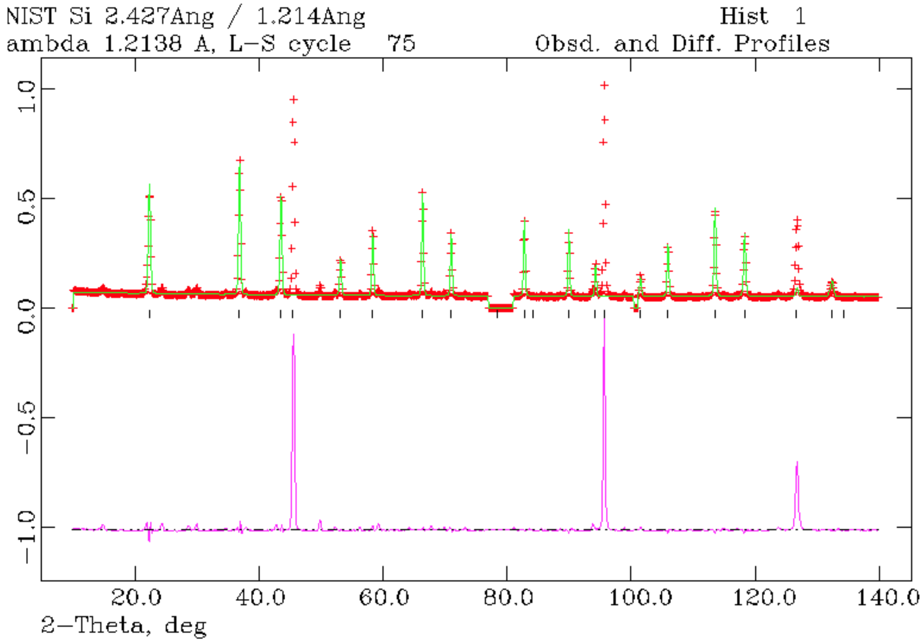


Science Drivers

- As current generation of instruments
- Chemical crystallography
  - $Q_{max} \sim 12.5$ Å^{-1}
  - Variable resolution
  - Trade flux for resolution
- Parametric studies
  - In-situ chemical processing
  - Fast kinetics
  - Phase diagram mapping
  - Complex/multi-role sample environments
- New Science?
  - Incoherent scattering separation/suppression
  - Elastic/QENS/inelastic options

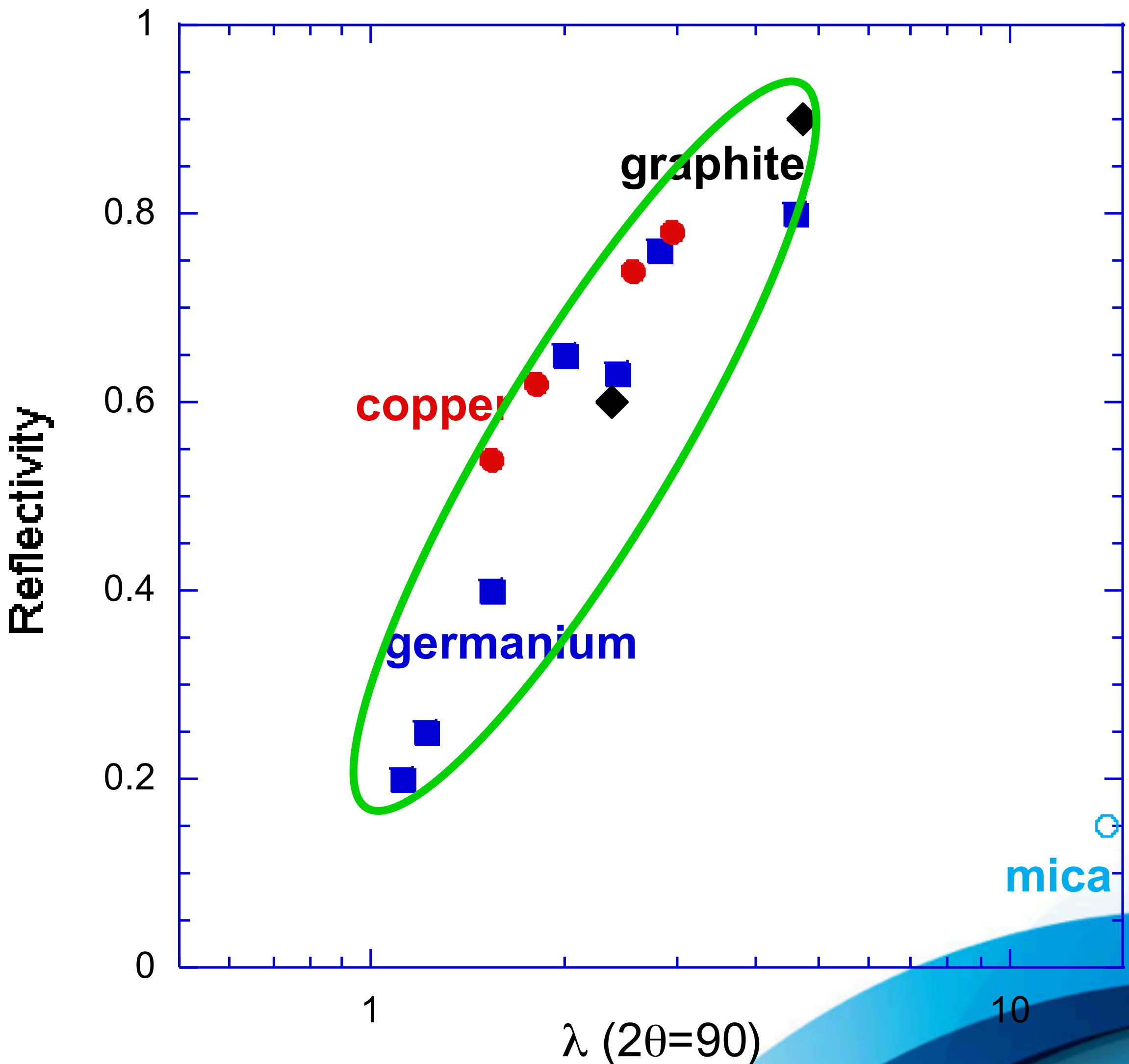
Monochromators



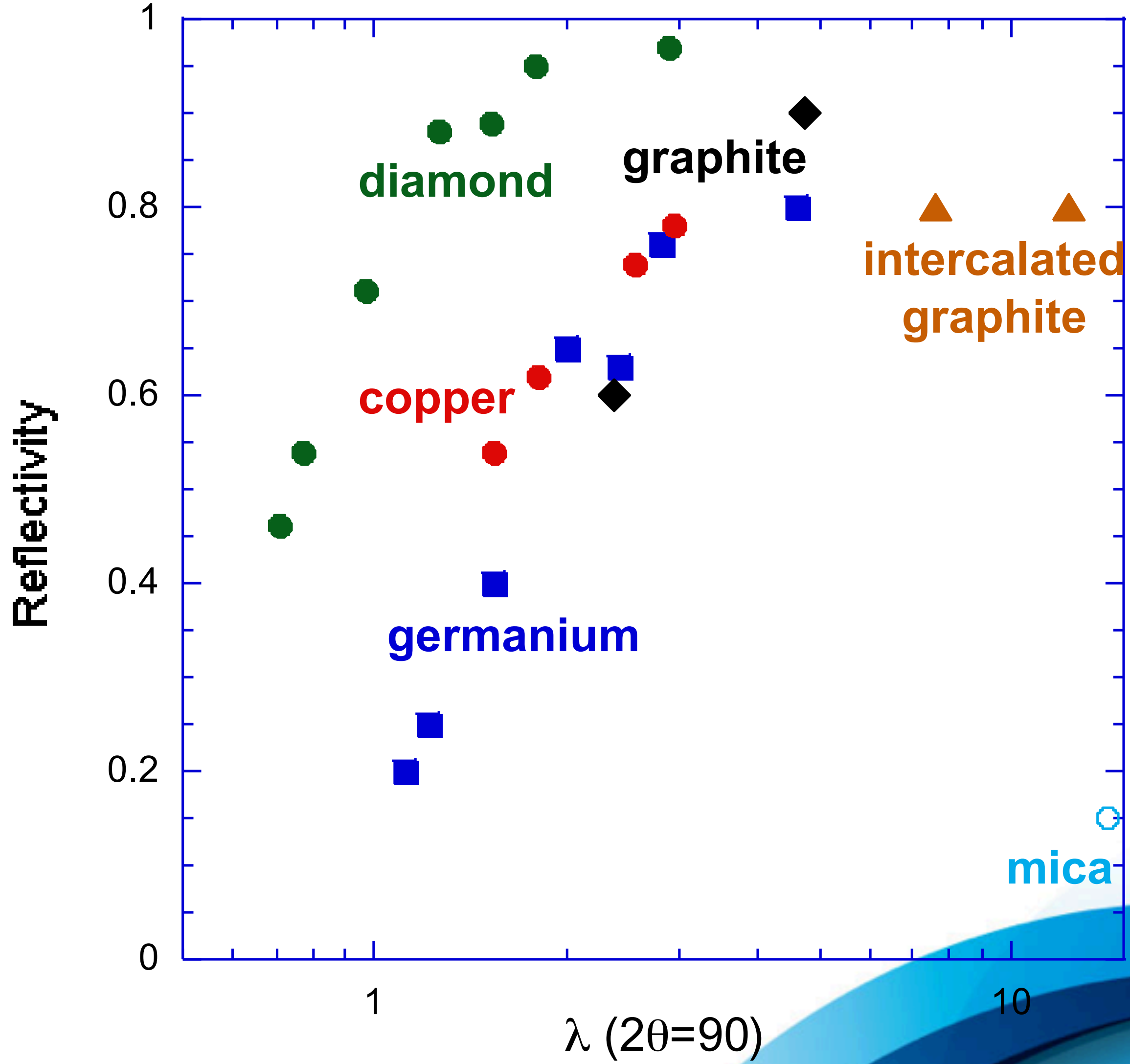


- Separate $\lambda/2$ and/or $\lambda/3$ as well as reflection coexistence in t-o-f- at detector
- Immediate gain in Q-range coverage
- Immediate gain in effective count rate

Monochromator materials



Monochromator materials



Detector

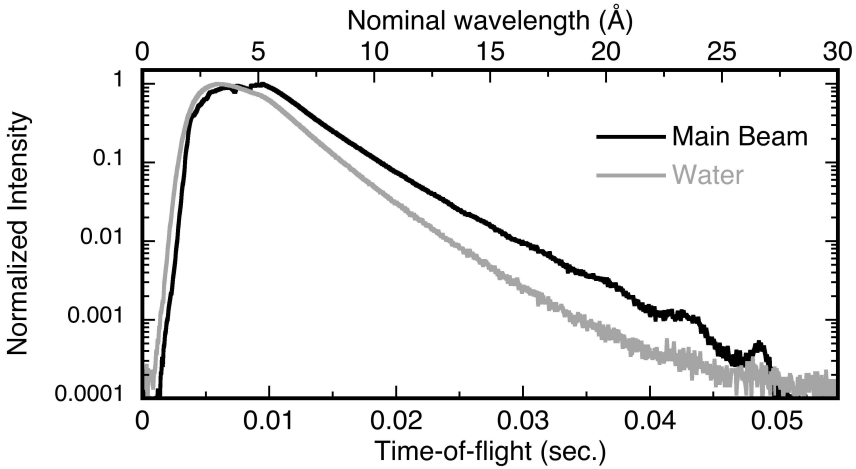
- Issue is limited/no? access to ^3He
- Investigate other technologies
  - Solid state boron thin films
  - Scintillation with wavelength shifting fibres
  - ZnS scintillators with PMTs?
- Event mode data collection offers advantages
  - Separate multi-wavelength data
  - Energy resolution
- Usability
  - Data visualisation/reduction familiar to users
  - Data format easily handled by existing software

New Capabilities

- Multi-wavelength data collection
  - Depends on instrument total length (e.g. 1 Å on 35 m instrument takes 9 ms, 1.8 Å takes 16 ms)
  - Developments in available monochromator types
  - Develop 'dirty' monochromators
  - Investigate sandwich monochromators
- Separate coherent/incoherent scattering
  - Depends on sample-detector distance
  - Sample temperature
  - Incident wavelength
  - Beam tailoring?
- Elastic/inelastic/QENS measurements
  - Depends on sample-detector distance
  - A PSC to tailor incoming pulse on monochromator
- Fast kinetic sampling measurements?
  - Sampling time around 4ms
  - Repetition rate 14 Hz

Incoherent scattering

Figures from A. Wildes (ILL)



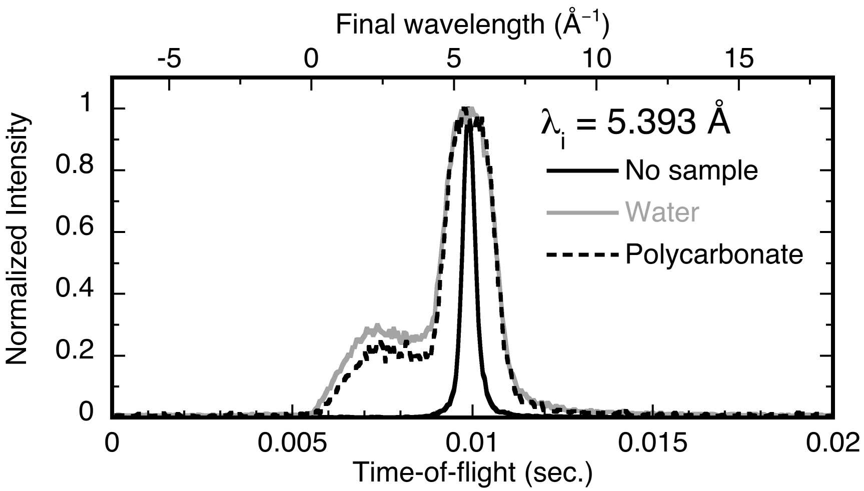
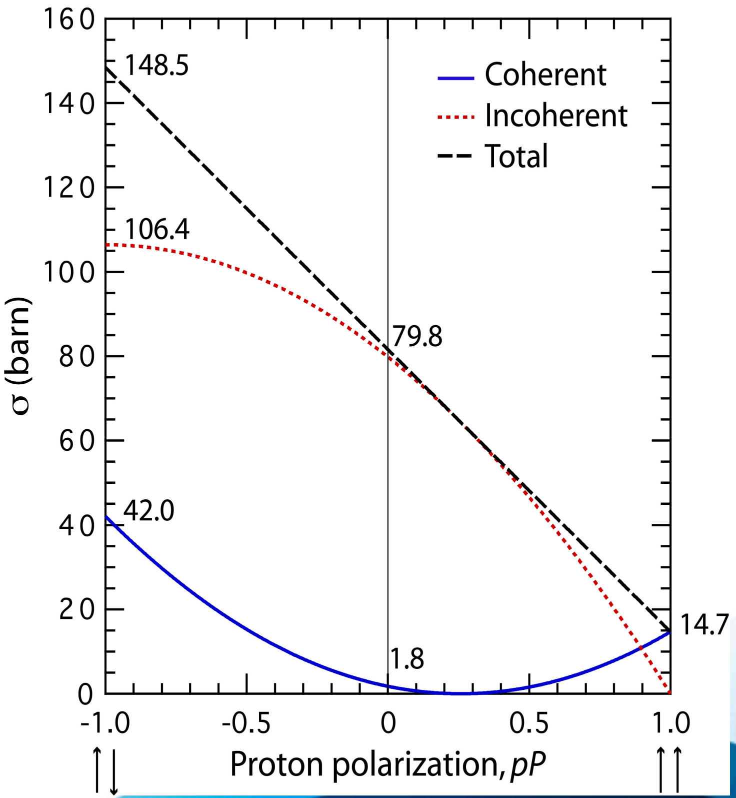


Figure from C. Carlile (ESS), M. Karlsson (Chalmers)



Inelastic scattering mapping

Challenge for ^{1}H measurement

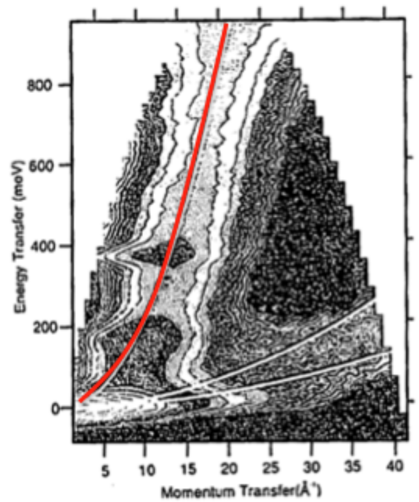
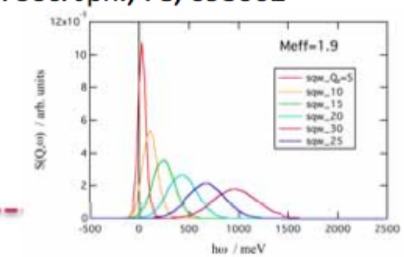


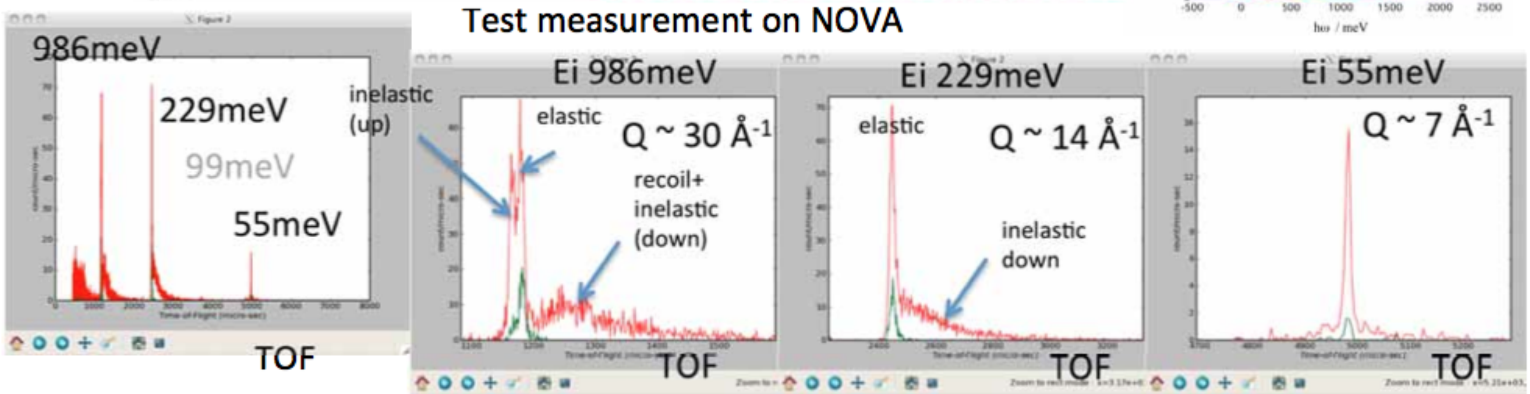
Fig. 1. $S(Q,\omega)$ map for a coal sample (sub-bituminous A) at 2 K containing ~5 wt% of H. Obtained with the MARI spectrometer (ISIS). Recoil lines for H, C and Al atoms are superimposed.

- Direct measurement of S(Q,E) by Femi-chopper
  - Monochromatic neutron with ΔE/Ei ~ 10%
  - Determination of effective mass
  - (Determination of excitation level)
  - Full use of event-mode: multi-Ei measurement
    - Nakamura et a. J. Phys. Soc. Jpn., 78, 093002 (2009)

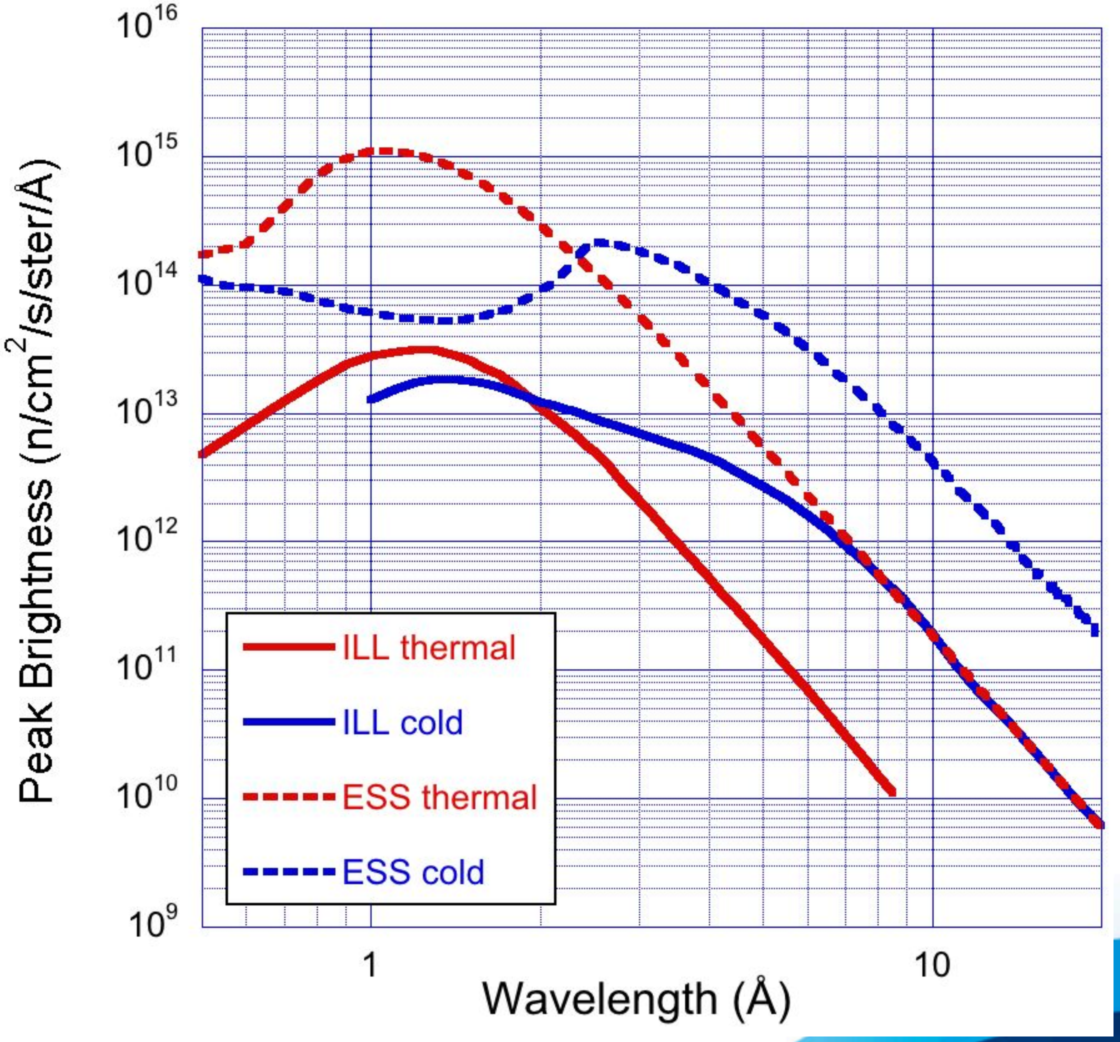
$$E_R = \hbar\omega_R = \frac{\hbar^2 Q^2}{2m^*}$$



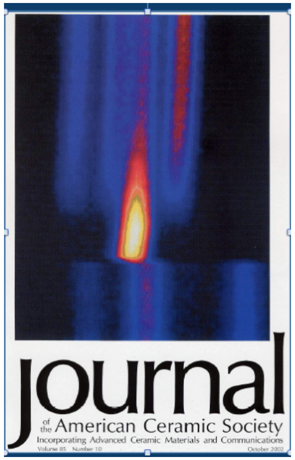
Test measurement on NOVA



Fast kinetics



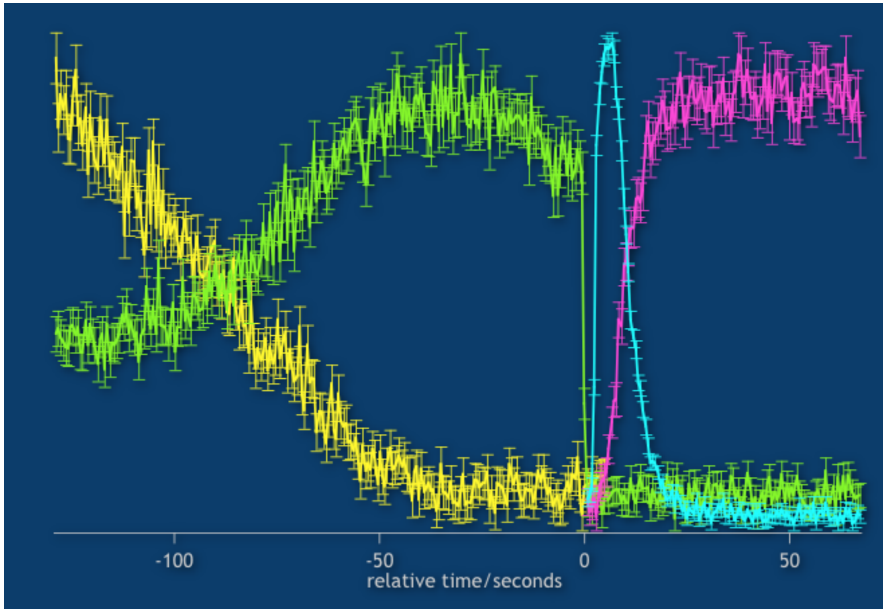
ms sampling?

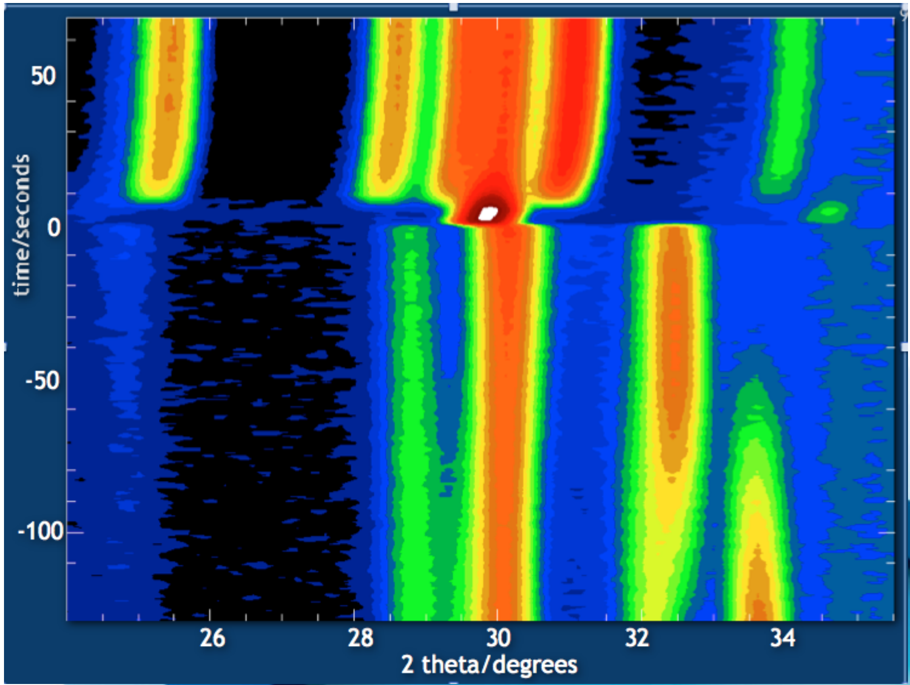


D.P. Riley, E.H. Kisi, T.C. Hansen, A. Hewat, *J. Am. Ceramic Soc.* **85** (2002) 2417-2424.

Data collection ~120 ms at 5-6 Hz
Histogram binned
Allows kinetic information to be extracted

What would be possible with 4ms data collection at 14 Hz coupled with event mode detection?





Summary

- Investigate an instrument based on monochromators
  - Simulate and optimise beam transport
  - Quantify feasibility of added value techniques
  - Compare with existing instruments
  - One instrument or several on guide
  - Detector development
  - Monochromator development
  - Begin development of sample environment
- Timeline
  - Post doc position
    - 2-year position
    - 50% science / 50% instrumentation
  - Instrument concept initial submission in 2013 (round 2)