ESS SANS - summary of conclusions of SANS Task group meeting, London, 16/2/01 and some subsequent discussions (revised 26/3/01)

Group members: R.K.Heenan (ISIS), R.Cubitt (ILL), K.Mortensen (Riso), D.Schwahn (Julich), A.Wiedenmann (Berlin). Further ideas have been contributed by F.Mezei (Berlin).

SANS is always a compromise between count rate, Q range and Q resolution. All three ESS neutron sources under discussion (50Hz, ~5MW; 10Hz ~1MW, and 16.67Hz long pulse ~5MW) would be suitable for some kind of SANS machine. It has been assumed in our discussions that a coupled hydrogen moderator on a 5MW ESS target has the same spectrum as the ILL cold source, currently the best in the world, and that the effect of neutron guides and/or benders would be the same in each case. **Future clarification of engineering details, such as scaling of moderator output with target power and detail comparison with ILL might alter the discussion here.**

Key features of pulsed source SANS are

(a) A wide simultaneous Q range in a single measurement, by using a broad range of λ. This gives a scientific opportunity e.g. for anisotropic scatterers, systems undergoing dynamic change and increasingly more complex multi-component samples. In such cases not having to move the detector improves the overall experiment. Data are well suited to model fitting or Fourier transform methods.

(b) Improved Q resolution over that given by a typical 10% reactor velocity selector. e.g. for "peaks" - lamellar phases, membranes, flux line lattice etc., and "wiggles" - detailed investigation of interfacial structures etc. by contrast variation, many of which are resolution limited at current reactor sources.

(c) Given the same or similar time averaged moderator spectra, the ESS pulsed source has count rate gains of a few up to ~10 times ILL by either simultaneously using more of the spectrum OR by increasing the repetition rate of the source with a smaller wavelength band and Q range. These **potential** gains, though useful, are not spectacular, thus the science case and complementarity of pulsed source against reactor SANS needs to be considered.

Single "figure of merit" comparison of ESS SANS with ILL SANS is NOT possible - neutrons are used in different ways - conclusions depend on the system under study and the science involved. We present counts at a given Q for a notional "flat scatterer" rather than a simple "flux at sample at a given λ" as used on reactors, though note most scatterers fall off steeply with Q, the pulsed source puts relatively more counts where signals are weaker.

1. The task group are agreed upon certain instrument characteristics for general purpose SANS, whilst they are not entirely in agreement over whether a 10Hz short pulse or 16Hz long pulse is best, in fact both would be good.

- A flexible instrument, "looking like D22" with a ~1m square detector moving from say 2m to >20m in a heavily shielded vacuum tank, in order to optimise, λ range, Q range, and geometric resolution to suit particular experiments. (e.g. crystalline materials such as metals might need to use only neutrons λ > 4 or 5 Å, above the Bragg cut-off). Incident collimation will require choppers to select wavelengths and remove frame overlap (out to λ ~ 30 Å) as well as the usual movable guide sections to change collimation length. The figures below illustrate some instruments with the sample at 21m (relatively far our, which suits the long pulse) and a detector at two extremes, 23m and 36m (λ_{max} ~ 11Å at 10Hz). Optimal sample positions and instrument lengths vary in practice with source repetition rate to avoid inconvenient prompt spikes and to select appropriate λ bands - thus comparisons should not be taken too literally.
- A coupled cold moderator, for highest flux.
- A guide/bender to remove the instrument from a direct view of the moderator fast neutron and prompt spike background, to give λmin ~ 2 Å (or possibly towards 1Å, await results at SNS). ESS prompt spike background will likely be pro-rata worse than at say ISIS. It would for now be unwise to need to have spikes in the longer λ part of the spectrum. (Fig 19 shows that the monitor prompt spike at ISIS is >20 times worse on CRISP, even after a T_0 chopper, than on LOQ after a bender.)
- Careful attention to shielding & collimation to improve signal/background over existing pulsed sources. Many SANS experiments are detector count rate limited, improved flux is most often used to measure smaller scattering cross sections.
- Individual run times will range from tens of seconds to hours. Rapid re-phasing of choppers to combine different data frames might be desirable at 50Hz.
- Generally the available Q range has to be "over specified" due to fall off in pulse source count rate at extremes of Q range. Accessible Q of 0.001 to 1.0 $Å^{-1}$ is required.

2. 1MW, 10Hz SANS- largest Δλ band gives best simultaneous Q ranges,(e.g. 0.002 to 0.1 $Å^{-1}$) loss of flux from lower power source is recovered by using spectrum down to λ ~ 2Å and in better overall experiment times. Inclusion of shorter λ close to beam stop worsens Q resolution due to a 1/λ term, though these can be omitted in final data reduction. At the smallest Q, longest λ , a 5MW source will always have more counts. At 10Hz backgrounds are least from the source & other beam lines; there is no prompt spike in data collection frame; a single chopper at ~6 -10m. Being forced to collect a wide Q range is good for many experimenters. Continuously varying Q

resolution and λ contributions are easier to deal with than combining data from different detector distances and/or wavelength bands. (At longer L_2 and longer λ could use time of flight to separate the 30 -50% inelastic component of supposed incoherent background from H_2O etc. thus improving signal/background for dilute samples.)

3. 5MW, 50Hz SANS, good count rates over very limited Q ranges particularly at longer distances, due to smaller $\Delta\lambda$, thus is most similar to a reactor. Will need three choppers in collimation section to remove frame overlap. Shortest possible guide/bender (higher background & worse constraints with neighbouring beams). 50Hz is worst for prompt spikes. Best suited to very short, high flux beam line. Removing pulses to operate at 25Hz or less expands Q range, but leaves prompt spike(s) in frame. How large these might be is uncertain, they will likely be much worse than at ISIS ?

4. 5MW, 16.67Hz long pulse. The 2msec long pulse time spread forces relatively long beam lines, with no short wavelengths used (which suits Bragg scatterers & polarising mirrors) to give good Q resolution. Count rates could be ~5 times better than 10Hz at smallest Q, ~2.5 times better in mid-Q, but overall Q range is half that at 10Hz. (Count rate gains could be eroded if moderator output does not scale linearly with target power.) At longer λ and longer path Q resolution is generally comparable to 10Hz. Building shorter path, long pulse, beam lines would however pose resolution problems. For the best λ range we have to count through a prompt spike of at present uncertain size, e.g. removing at least 9.9-10.5Å at 24m, or 6.6-7.0Å at 36m. Inelastic scatter, separated by time-of-flight, further restricts the λ range at long sample-detector at 16.67 Hz and 50Hz for hydrogenous samples.

(R.K.Heenan, Revised 27/2/01, after SANS task group meeting in London)

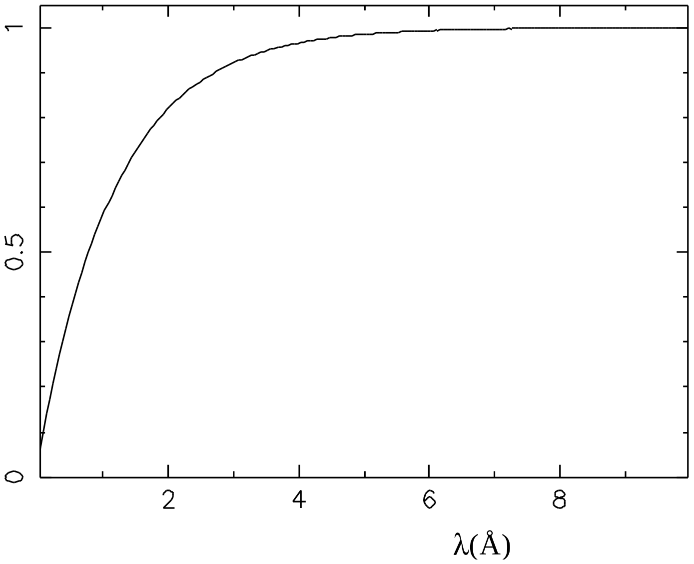

Fig.1. "Detector efficiency" assumed (~ 1mm thick scintillator plus 5mm aluminium) in all calculations. No further allowance has been made for neutron guide or sample transmissions.

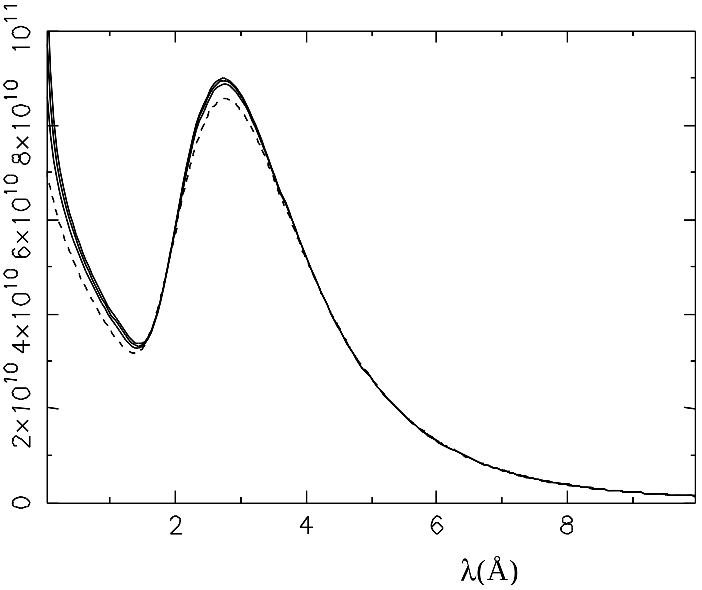

Fig.2(b) Coupled liquid H_2 moderator, simulated monitor spectra using efficiency in Figure 1, at 5(dashed), 10, 15 and 25m, using t_0=300μsec, neutrons/cm^2/sec/Å/sterad per pulse

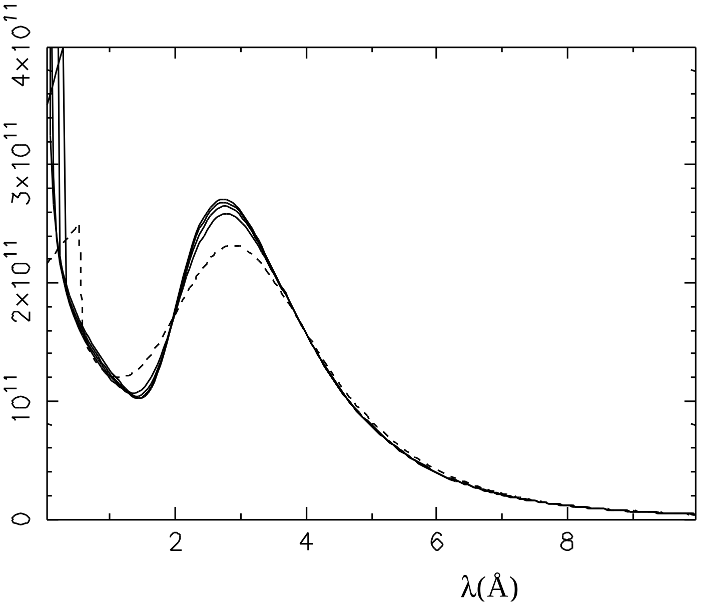

Fig.2(c) 2msec Long pulse, coupled liquid H_2 moderator, simulated monitor spectra at 5(dashed), 10, 15, 25 and 100m, using t_0=1300μsec, neutrons/cm^2/sec/Å/sterad per pulse

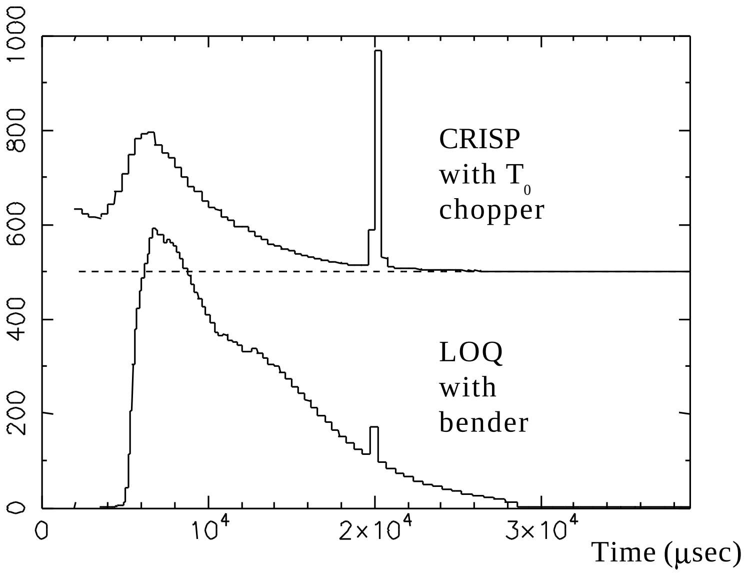

Fig 19. ISIS monitor spectra at 25Hz on CRISP reflectometer (displaced) & LOQ at ~10m. LOQ has bender and wavelength selecting chopper (λ ~ 2 -10 Å), CRISP has T_0 chopper (10cm ?) and wavelength selecting chopper. Runs have same length and similar width bins at 20msec, but scintillator detector types and beam sizes are different. CRISP is probably more efficient at short λ but has lost flux at long λ due to air paths. Despite T_0 chopper CRISP spike makes monitor spectrum (and reflection measurements) impossible. "Prompt pulses" at 20 and 40msec are *still* significant on LOQ, where note also aluminium Bragg dips due to beam line vacuum windows.

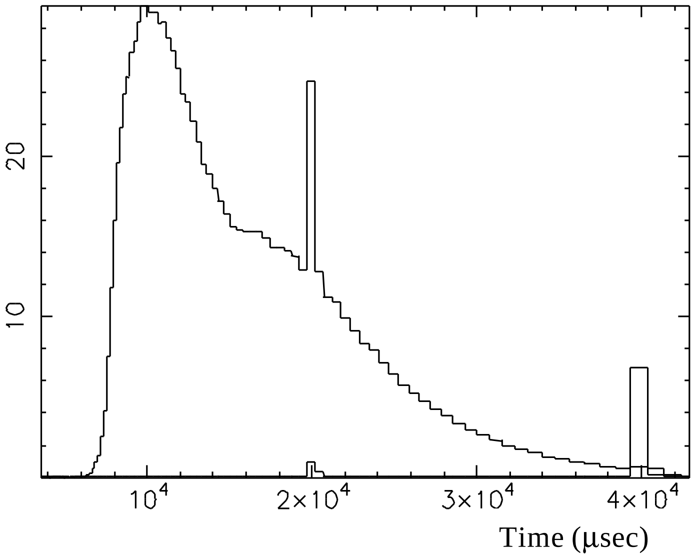

Fig 20. LOQ at ISIS, λ = 2-10Å spectrum from 1mm H2O scattering, summed over 64cm square detector at 15.1m. The second prompt pulse prevents counting through the frame boundary, limiting the longest wavelength to 10Å at this distance.

The prompt spike is located mainly to the fast neutron, un-bent beam, side of the beam stop. This may be due to a weakness in the current beam line collimation on LOQ.

The small *lower trace* is a "shutter closed" contribution in which the spike is now uniformly spread over the detector. The baseline (invisible here) is the same as the intrinsic detector background measured with ISIS off (0.28 cts/cm^2/hour). Note that we need to measure cross sections ~1% of 1mm H2O, thus this spike and its tail are still significant. A minimum of 300mm of borated paraffin wax shielding covers the detector, else the prompt spike increases by orders of magnitude. (The opening edge of the chopper is showing inelastic scattering, neutrons accelerated by the sample arrive early at the detector.)

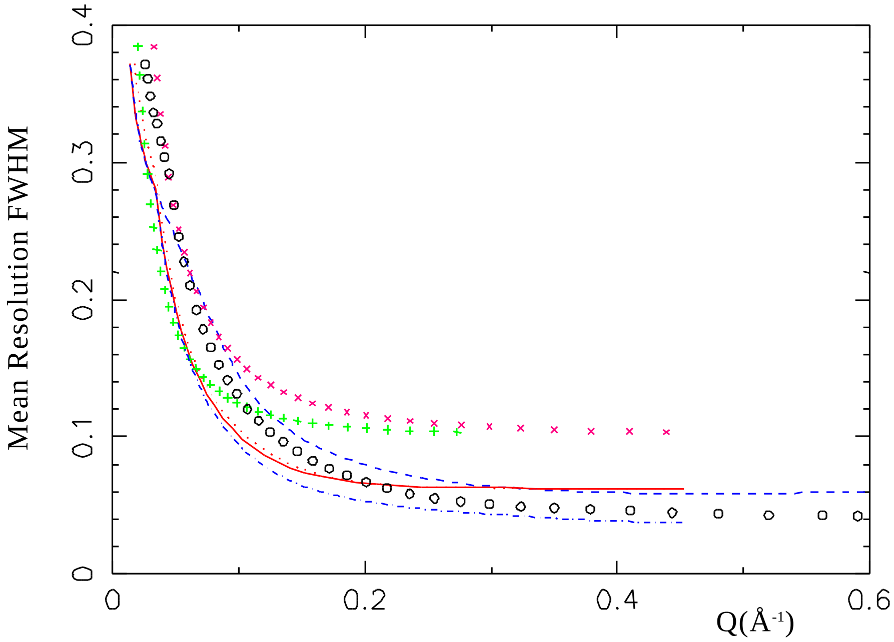

Fig.21 At 24m (19/2/2), δQ/Q, FWHM resolution (Gaussian approximations, compare more accurate results of Figure 23.) coupled H_2 moderator, 10mm diameter sample.

Line - λ = 4.6-12Å, 5MW, 16.67Hz, long pulse
Dots - λ = 4.6-9.9Å, (the same, but stopping before prompt spike at 9.9Å),
Circles -λ = 3.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 9.9Å, 5MW, 50Hz
Dashes - λ = 2-12Å, 1MW, 10Hz (full Q range truncated here),
Dot-Dash - λ = 4.6-12Å, 1MW, 10Hz (improve resolution by omitting short λ near beam stop),
xxx - λ = 5Å, 10% FWHM, "ILL reactor"
+++ - λ = 8Å, 10% FWHM, "ILL reactor"

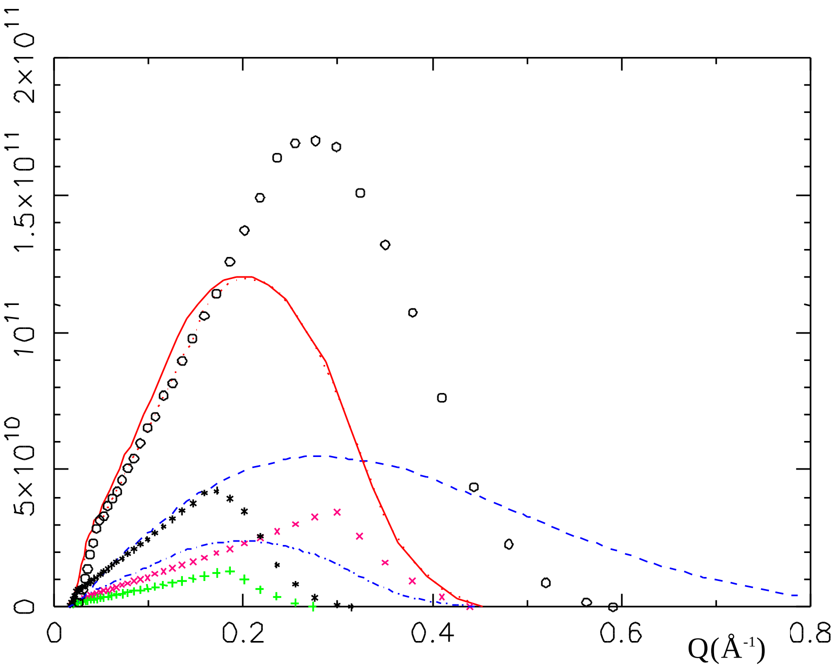

Fig. 22(a) At 24m (19/2/2), 1cm^{-1} flat scatterer, coupled H_2 moderator, 1m square detector at 2m sample-detector (assuming perfect neutron guide brings source to 19m).

Line - λ = 4.6-12Å, 5MW, 16.67Hz, long pulse
Dots - λ = 4.6-9.9Å, (the same, but stopping before prompt spike at 9.9Å),
Circles - λ = 3.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 9.9Å, 5MW, 50Hz
Dashes - λ = 2-12Å, 1MW, 10Hz
Dot-Dash - λ = 4.6-12Å, 1MW, 10Hz
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"

(Calculations are numerical integrations over detector and spectrum, assuming $L_1 = L_2$, $R_1 = 2R_2$, detector FWHM ΔR = 12mm, Rmin = 2.5 x penumbra)

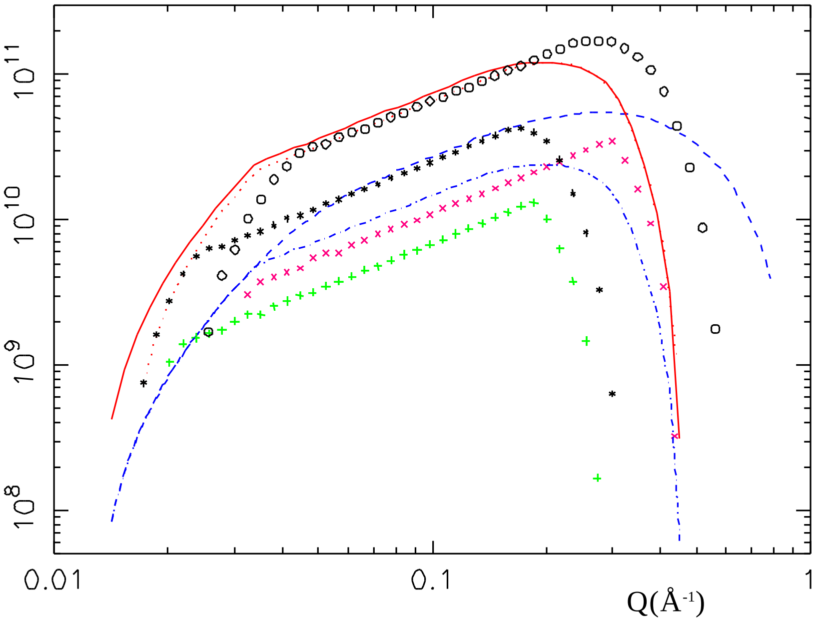

Fig. 22(b) At 24m (19/2/2), 1cm^{-1} flat scatterer, coupled H_2 moderator, 1m square detector at 2m sample-detector (assuming perfect neutron guide brings source to 19m).

Line - λ = 4.6-12Å, 5MW, 16.67Hz, long pulse
Dots - λ = 4.6-9.9Å, (the same, but stopping before prompt spike at 9.9Å),
Circles - λ = 3.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 9.9Å, 5MW, 50Hz
Dashes - λ = 2-12Å, 1MW, 10Hz (with this λ range at 10Hz a longer sample-detector might be better),
Dot-Dash - λ = 4.6-12Å, 1MW, 10Hz
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"

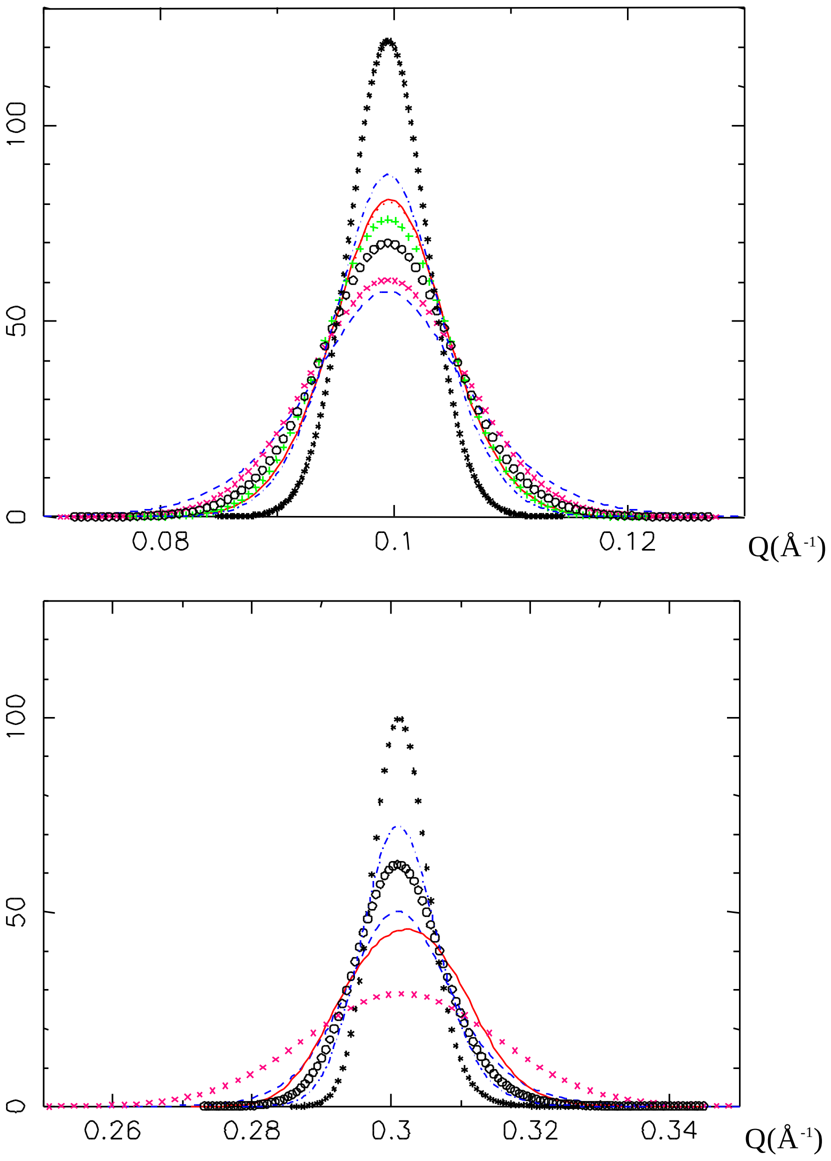

Fig. 23. At 24m (19/2/2), more accurate Q resolution at Q=0.1 and Q =0.3 Å^{-1} (Sum of Gaussians convoluted with moderator emission times). At Q =0.3 long pulse is more asymmetric than 10Hz short pulse despite simple mean in Fig 21 suggesting they should be the same.

Line - λ = 4.6-12Å, 5MW, 16.67Hz, long pulse
Circles - λ = 3.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 9.9Å, 5MW, 50Hz
Dashes - λ = 2-12Å, 1MW, 10Hz
Dot-Dash - λ = 4.6-12Å, 1MW, 10Hz
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"

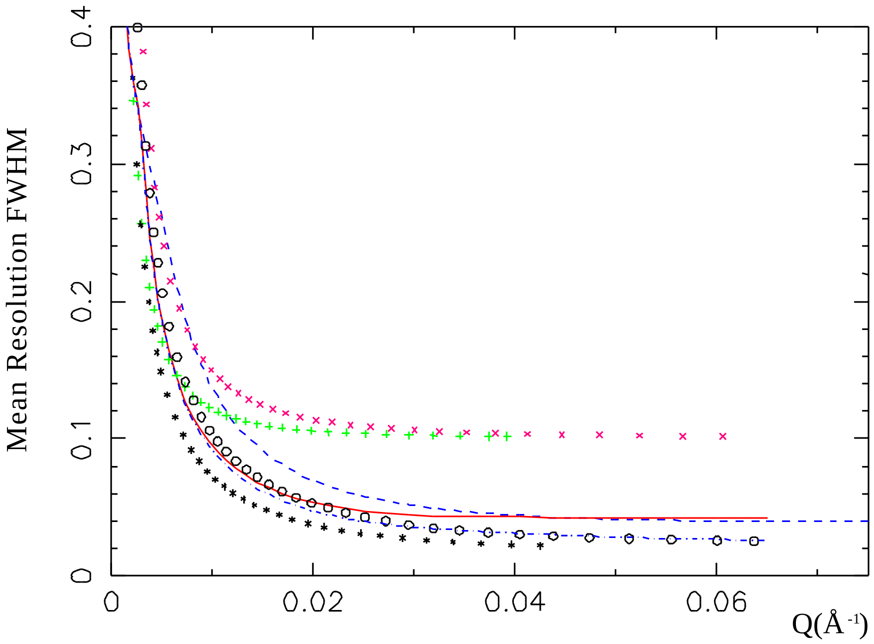

Fig.24 At 36m (6/15/15), δQ/Q, FWHM resolution (Gaussian approximations) coupled H_2 moderator, 6mm diameter sample.

Line - λ = 4.4-11Å, 5MW, 16.67Hz, long pulse (Prompt spike at λ=6.6 - 7.0 Å is still included here),
Circles -λ = 4.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 8.8Å, 5MW, 50Hz
Dashes - λ = 2-11Å, 1MW, 10Hz (full Q range truncated here),
Dot-Dash - λ = 4.4-11Å, 1MW, 10Hz (improve resolution by omitting short λ near beam stop)
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"

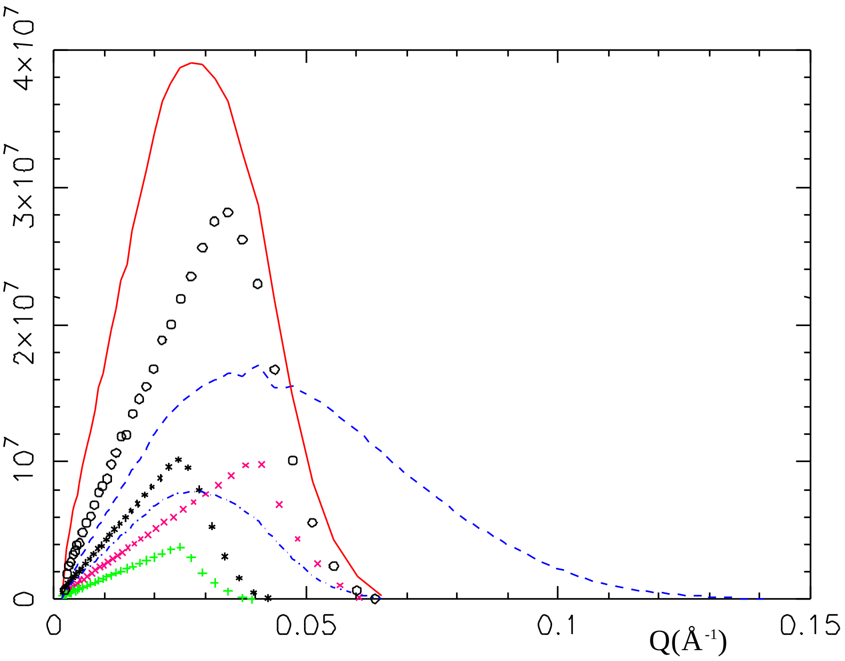

Fig. 25(a) At 36m (6/15/15), 1cm^{-1} flat scatterer, coupled H_2 moderator, 1m square detector at 15m sample-detector, 6mm diameter sample.

Line - λ = 4.4-11Å, 5MW, 16.67Hz, long pulse (Prompt spike at λ=6.6 - 7.0 Å is still included here **Inelastic scatter separated by time-of-flight** from hydrogenous samples would limit the λ range to 4.4 - 9.6 or 7.6 - 11.0 Å),
Circles -λ = 4.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 8.8Å, 5MW, 50Hz
Dashes - λ = 2-11Å, 1MW, 10Hz
Dot-Dash - λ = 4.4-11Å, 1MW, 10Hz
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"

λ ranges here are accurate, with optimistic 1.5msec (short pulse) and 3.5 msec (long pulse) allowed for spikes at frame boundaries.

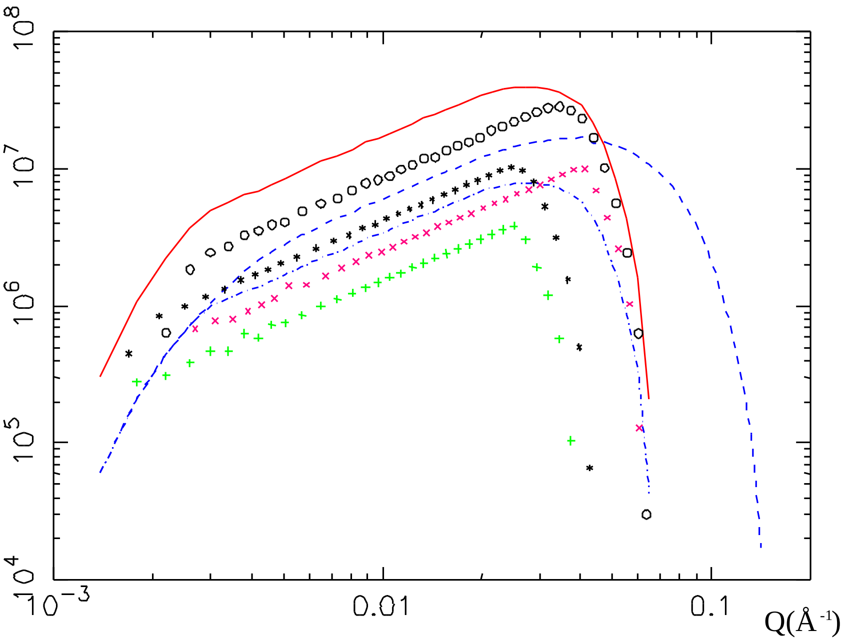

Fig. 25(b) At 36m (6/15/15), 1cm^{-1} flat scatterer, coupled H_2 moderator, 1m square detector at 15m sample-detector

Line - λ = 4.4-11Å, 5MW, 16.67Hz, long pulse (Prompt spike at λ=6.6 - 7.0 Å is still included here. **Inelastic scatter separated by time-of-flight** from hydrogenous samples would limit the λ range to 4.4 - 9.6 or 7.6 - 11.0 Å),
Circles -λ = 4.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 8.8Å, 5MW, 50Hz
Dashes - λ = 2-11Å, 1MW, 10Hz (full Q range truncated here),
Dot-Dash - λ = 4.4-11Å, 1MW, 10Hz
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"

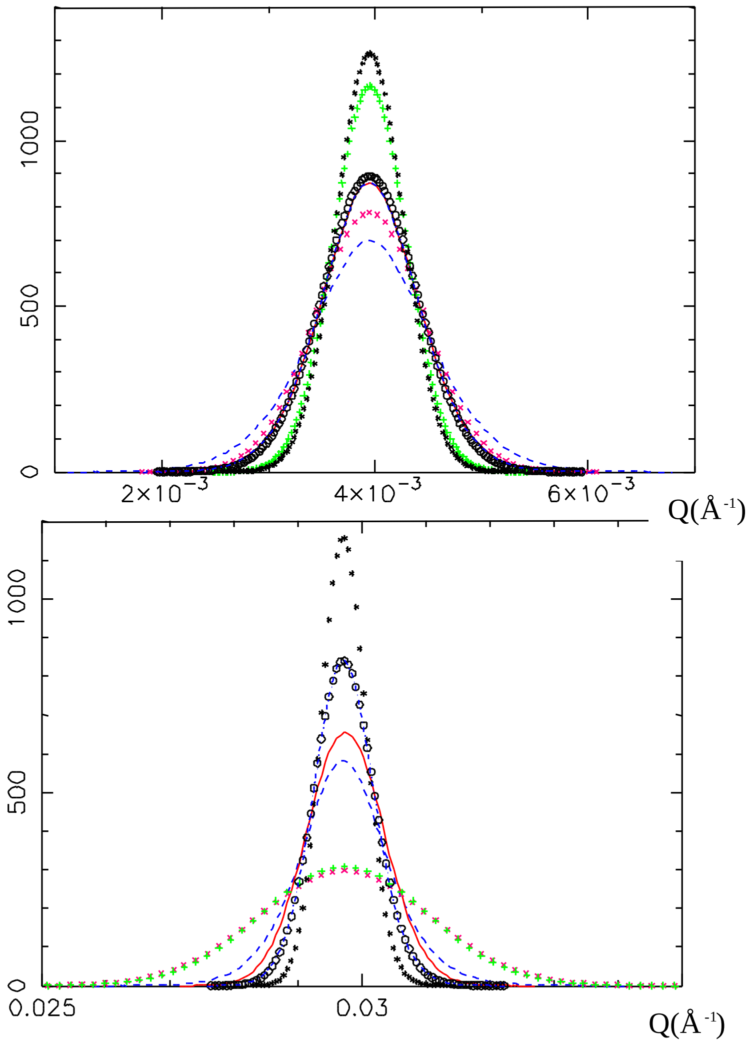

Fig. 26 At 36m (6/15/15),), more accurate Q resolution at Q=0.004 and Q =0.03 Å^{-1} (Sum of Gaussians convoluted with moderator emission times.) Shorter λ always worsens resolution, but can be omitted near beam stop during data reduction, with minimal effect on counts.

Line - λ = 4.4-11Å, 5MW, 16.67Hz, long pulse
Circles -λ = 4.6-6.6Å, 5MW, 50Hz
Asterisk -λ = 6.8 - 8.8Å, 5MW, 50Hz
Dashes - λ = 2-11Å, 1MW, 10Hz
Dot-Dash - λ = 4.4-11Å, 1MW, 10Hz
xxx - λ = 5Å, 10% FWHM, , "ILL reactor"
+++ - λ = 8Å, 10% FWHM, , "ILL reactor"