SANS Instruments

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Small angle neutron scattering is a well established technique to examine structures on a distance scale of say 10 to 1000 A. SANS was initially developed at fixed wavelength reactor sources and for detector-sample distances mainly between 1 and 20m. The advantages of pulsed source SANS using white beam, time-of-flight have not yet been widely appreciated, despite the presence of several good instruments on existing pulsed sources. For historical reasons these existing instruments have relatively short, fixed, flight paths. The key feature of SANS at the ESS is to be able to build flexible instruments with movable detectors that will allow an optimisation of Q range, count rate and Q resolution on an experiment by experiment basis. At lower pulse repetition rates time of flight allows a wide simultaneous Q range at a single setting of the instrument, suited to dynamic or anisotropic systems. At higher repetition rates considerably greater count rates may be achieved over a more limited Q range, with the detector being moved similar to present reactor instruments or perhaps the wavelength band changed in order to expand the Q range.

All three ESS neutron sources under discussion (50Hz, ~5MW; 10Hz ~1MW, and 16.6Hz long pulse ~5MW) would be suitable for SANS, and would in many aspects be superior to D22 at the ILL which is presently the best SANS instrument in the world. As illustrated below the 16.6Hz long pulse plus the 50Hz ~5Mw should be the best choice for the two target stations provided one also considers operation at sub-multiples of 50Hz for a wider simultaneous Q range.

Significant new experimental opportunities for SANS will arise with count rates up to an order of magnitude higher than presently available, wider simultaneous Q ranges and improved Q resolution.

It has been assumed in our discussions that a coupled hydrogen moderator on a 5MW ESS target has the same time averaged spectrum as the ILL cold source and that the effect of neutron guides and/or benders would be the same in each case.

Future clarification of engineering details, such as the optimisation of neutron output for given target power and moderator layout might alter the outcome of the discussion here.

Key features of pulsed source SANS

Given similar time averaged moderator spectra, the ESS pulsed source has count rate gains of a few up to ~10 times D22 at the ILL the current world best. This may be achieved at lower pulse repetition rate by simultaneously using more of the spectrum OR at higher repetition rates with a smaller wavelength band and smaller Q range. These potential gains will provide new experimental opportunities for SANS.

Best in world count rates.

New opportunities for SANS experiments.

Single "figure of merit" comparison of ESS SANS with reactor SANS is NOT possible – neutrons are used in different ways - conclusions depend on the system under study and the science involved. We present (Fig. 3 and 4) 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. Since many scatterers fall off steeply with Q, the pulsed source puts relatively more counts where signals are weaker.

Simple comparison with reactor generally not possible.

Some experiments need to optimise the instrument for highest flux in a given Q-range, other experiments might optimise for highest resolution (δQ/Q), and others may optimise for maximum available Q-range, even using the low-flux limits. A flexible instrument, "looking like D22" with as a *minimum requirement* a ~1m square detector moving from say 2m to 20m in a vacuum tank, in order to optimise λ range, Q range, and geometric resolution to suit particular experiments, e.g. only neutrons λ > 4 or 5 Å might be used with crystalline materials, above the Bragg cut-off, or when polarized neutrons are used. Dynamical studies require a large Q range in a single shot. 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 two instrumental set-ups with the sample at 21m (relatively far out, which suits the long pulse) and a detector at two extremes, 23m and 36m (λ_{max} ~ 11Å at 10Hz).

Flexible instrumentation.

If the use of a guide/bender and sufficiently good shielding allows operation at sub-multiples of 50Hz for wider simultaneous Q ranges, then the 16.6Hz long pulse and the 50Hz ~5MW sources might be the best scenario for the two target stations.

SANS possible on all proposed ESS sources.

In many experiments a wide simultaneous Q range in a single measurement, by using a broad range of λ will be important. The wider Q range offered by the pulsed source will present new scientific opportunities 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 quality. Data are well suited to model fitting or Fourier transform methods.

Wide simultaneous Q range - suits complex experiments & data fitting.

SANS instruments can be proposed to give improved Q resolution ($\delta Q/Q$) over that given by a typical velocity selector on a reactor. This will improve data for "peaks" - in 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.

Improved Q resolution.

A coupled cold moderator is preferred for highest flux. The longer time constants of coupled moderators do not unduly degrade Q resolution (except for very short flight paths at short λ).

Coupled cold moderator.

A guide/bender is absolutely necessary to remove the instrument from a direct view of the moderator fast neutrons and prompt spike background, to give a λ_{min} ~ 2 Å (or possibly towards 1 Å, await results at SNS). Fig. 2 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.

Indirect view of moderator is essential.

Careful attention has to be given to shielding & collimation for a sufficiently good signal/background. Improved flux is most often used to measure smaller scattering cross sections. Many SANS experiments are detector count rate limited; there is an essential need for larger, faster detectors, with good stability and 5 -10mm pixel size.

Shielding for good signal/background is essential.

Faster, larger detectors needed.

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.

Rapid chopper re-phase may be useful.

Generally the available Q range has to be "over specified" due to fall off inherent to pulse sources of the count rate at the extremes of the Q range. Accessible Q of 0.001 to 1.0 $Å^{-1}$ is required.

"Over specify" the Q range.

ESS SANS - generic instruments

State of the art instruments would "look like D22 at the ILL", see Figure 1, with a large area detector of high-count rate capability, moving inside a heavily shielded vacuum tank. A 1m x1m multi-wire gas detector is the present best but development of larger and particularly faster detectors is important. The detector should be able to be offset from the beam axis to further enhance Q range when needed. There is no reason other than cost why even with present technologies a still larger detector area and vacuum tank could not be used. (Compare the success in other fields of MAPS and GEM at ISIS with up to 16m^2 of detector!) Having all detectors movable is a key feature, they are far easier to calibrate and normalise, as well as providing flexibility in SANS experiment design. Static "fixed banks at high Q" should be as far as possible avoided.

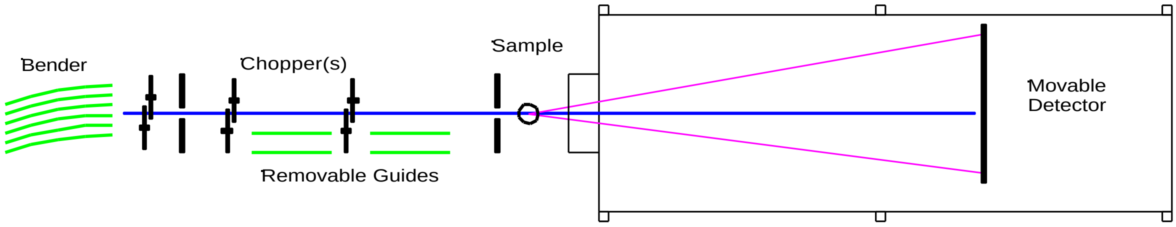

Fig. 1: Generic SANS instrument for ESS. Curved guide and/or bender removes beam from direct view of moderator. Large area detector (at least 1m x1m) moves in vacuum tank, and may be offset sideways. Substantial beam line and vacuum tank shielding will be required.

The incident guide/bender and beam collimation should be designed to provide collimation to match the longest sample-detector distance, with removable guide sections to bring the effective source closer to the sample for shorter sample-detector positions to give the usual $L_1 = L_2$. The need to use a curved guide and/or bender to remove fast neutrons, which later moderate inside the instrument, cannot be overstated, and is illustrated in Figure 2. One or more double disc choppers (three at 50Hz) will be needed to define the λ band used from each pulse, to remove frame overlap, and to completely remove pulses to work at lower repetition rates. At long sample-detector distance inelastic scatter, separated by time-of-flight, could further restricts the λ range; neutrons accelerated at the sample arrive very rapidly at the detector, possibly swamping the weaker signal from the end of the previous pulse. Inclusion of short λ, below the Bragg cut-off (~4 Å) can cause problems from multiple Bragg scattering and requires care in the use of crystalline materials for beam windows.

A typical configuration might be 6/15/15, a 36m long beam line with 6m guide/bender to remove direct view of moderator, 15m of collimation (plus removable straight guide sections) and finally a 15m vacuum tank. The longer the overall length of the beam line the smaller the λ range available (λ (Å) ~ 4T (msec)/L (m)) but the better is the $\delta\lambda/\lambda$ resolution, Given sufficient resources a further, shorter beam line (c.f. the old D17 at the ILL) might be attractive (at 50Hz, but not for the long-pulse). At a reactor SANS instrument per-

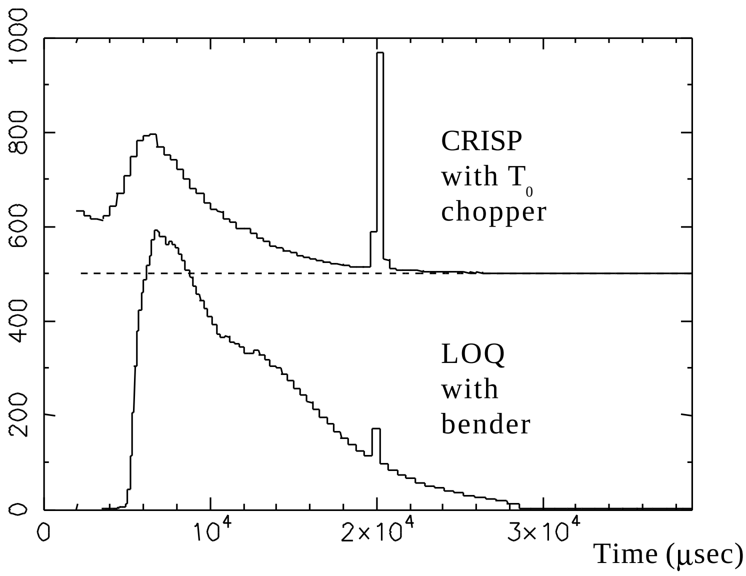

Fig 2: ISIS monitor spectra at 25Hz on CRISP reflectometer (displaced) & LOQ at ~10m. LOQ has bender and wavelength selecting chopper (λ ~ 2 -10 Å), CRISP has T_0 chopper (10cm ?) and wavelength selecting chopper. Runs have same length and similar width bins at 20 msec, but scintillator detector types 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 40 msec are *still* significant on LOQ, where note also aluminium Bragg dips due to beam line vacuum windows.

formance can be surmised from the neutron flux of a given wavelength arriving at the sample coupled with the sample-detector distance. On a pulsed source a range of wavelengths arriving at *different* radii on the detector may reach some given Q value, so that comparisons are not straightforward. Thus we compare scattering from a notional "flat scatterer" or some other scattering law as may be appropriate. Even such comparisons are difficult as count rate varies with the inverse fourth power of Q resolution (δQ/Q) which itself varies inversely with wavelength λ. The Table and Figures below compare some "typical" SANS instrument configurations, which are not necessarily optimal for the individual source repetition rates, but do provide a basis for discussion.

SANS at 16.6Hz long pulse, ~5MW

The 2msec long pulse time spread forces relatively long beam lines, with no short wavelengths used (which suits Bragg scatterers) in order to give wavelength resolution $\Delta\lambda_{fwhm}/\lambda$ better than the usual ~10%. This broadening also affects incident beam monitor spectra prior to the sample, and alters the band-pass of disc choppers. The data in Figures 3b and 4b show that with suitable compromises in instrument design (long beam line with no short wavelengths) the Q resolution from the long-pulse remains as good as that from the short pulse.

Count rates from the long pulse source are clearly the best due to ~3 times as many neutrons per proton pulse. Overall Q range is about half that at 10Hz and gains at high Q are not so good as the

Table 1. Approximate Q ranges for short & long L_2 SANS instrument case studies.

At 23m, L_2 = 2m (19/2/2), 10mm sample	**T_P msec**	**Notes**	**Simultaneous l range* (Å)**	**Q range$ ($Å^{-1}$)**
50Hz, 5MW	20 msec		3.6 - 6.6	0.026 - 0.57
"	"		6.8 - 9.9	0.017 - 0.30
16.6Hz, 5MW	62.5 msec		4.6 - 12	0.014 - 0.45
"	"	Avoid prompt spike	4.6 - 9.9	0.017 - 0.45
10Hz, 1MW	100 msec		2 - 12	0.014 - 0.79
"	"	Avoiding Bragg	4.6 - 12	0.014 - 0.45
Reactor 10% fwhm			5	0.033 - 0.43
Reactor 10% fwhm			8	0.020 - 0.26
At 36m, L_2 = 15m (6/15/15), 6mm sample				
50Hz, 5MW	20 msec		4.6 - 6.6	0.0022 - 0.062
"	"		6.8 - 8.8	0.0016 - 0.042
16.6Hz, 5MW	62.5 msec	Avoid inelastic@	4.4 - 9.2	0.00155 - 0.066
10Hz, 1MW	100 msec		2 - 11	0.0013 - 0.145
"	"	Avoid Bragg	4.4 - 11	0.0013 - 0.066
Reactor 10% fwhm			5	0.0026 - 0.059
Reactor 10% fwhm			8	0.0017 - 0.038

*Note λ range is restricted to >2 Å (guide cut off) and λ < 12 Å (sample transmission) and may be further restricted by time frame T_Π, prompt pulses and inelastic scatter from hydrogenous samples.

$ Detector is assumed $1m^2$, centred on the beam, with isotropic scatterer, else divide Q_{max} by v2, or increase Q_{max} if detector is offset. Minimum detector radius ~ 2.5 x penumbra.

@ Could use at other extreme, with reduced count rate, λ = 7.5 - 11.0 Å, (Q = 0.0013 - 0.038 $Å^{-1}$), or some intermediate range between these.

peak flux of the spectrum is not available unless poor resolution can be tolerated. (Using say λ < **4** Å the Q resolution curves would broaden assymetrically to high Q.)

For the best λ range at 16.6Hz we have to count through a prompt spike of at present uncertain size, e.g. removing at least 9.9-10.5 Å at 23m, or 6.6-7.0 Å at 36m.

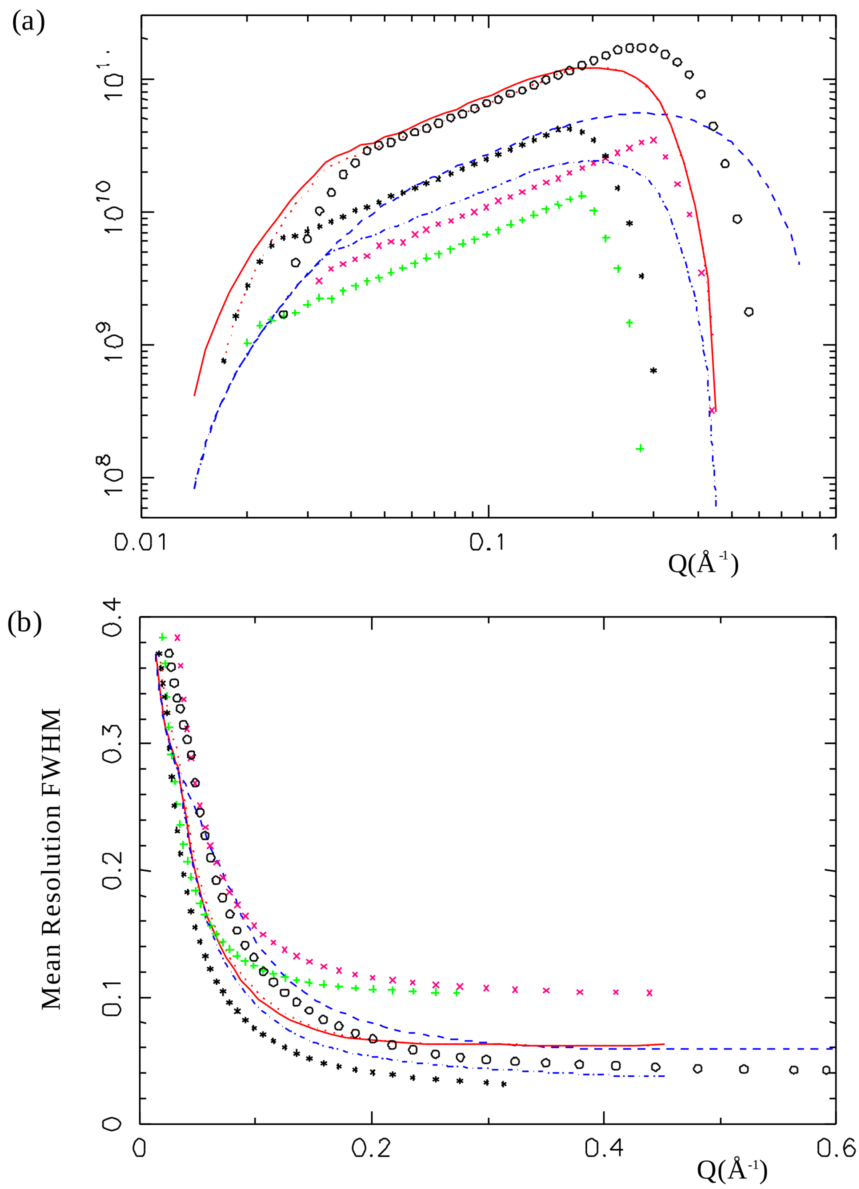

Fig.3: ESS - SANS At 23m (19/2/2), (a) 1cm^{-1} flat scatterer ,(b) $\delta Q/Q$, FWHM resolution coupled H_2 moderator, 10mm diameter sample.

line - λ = 4.6-12 Å, 5MW, 16.6Hz, long pulse
dots - λ = 4.6-9.9 Å, (stopping before prompt spike at 9.9 Å),
circles -λ = 3.6-6.6 Å, 5MW, 50Hz
asterisk -λ = 6.8 - 9.9 Å, 5MW, 50Hz
dashes - λ = 2-12 Å, 1MW, 10Hz (full Q range truncated in(b)),
dot-dash - λ = 4.6-12 Å, 1MW, 10Hz (improve resolution by omitting short λ near beam stop),
xxx - λ = 5 Å, +++ - λ = 8 Å, 10% FWHM, ~ "ILL reactor" assuming all other factors equal.

(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. A "1mm scintillator" detector efficiency has been included to make a realistic reduction of the short λ contribution. $\delta Q(FWHM)/Q$ is a simple mean of Gaussian approximations, actual resolution curves tend to have a relatively sharp peak and, where shorter λ are included, broader tails)

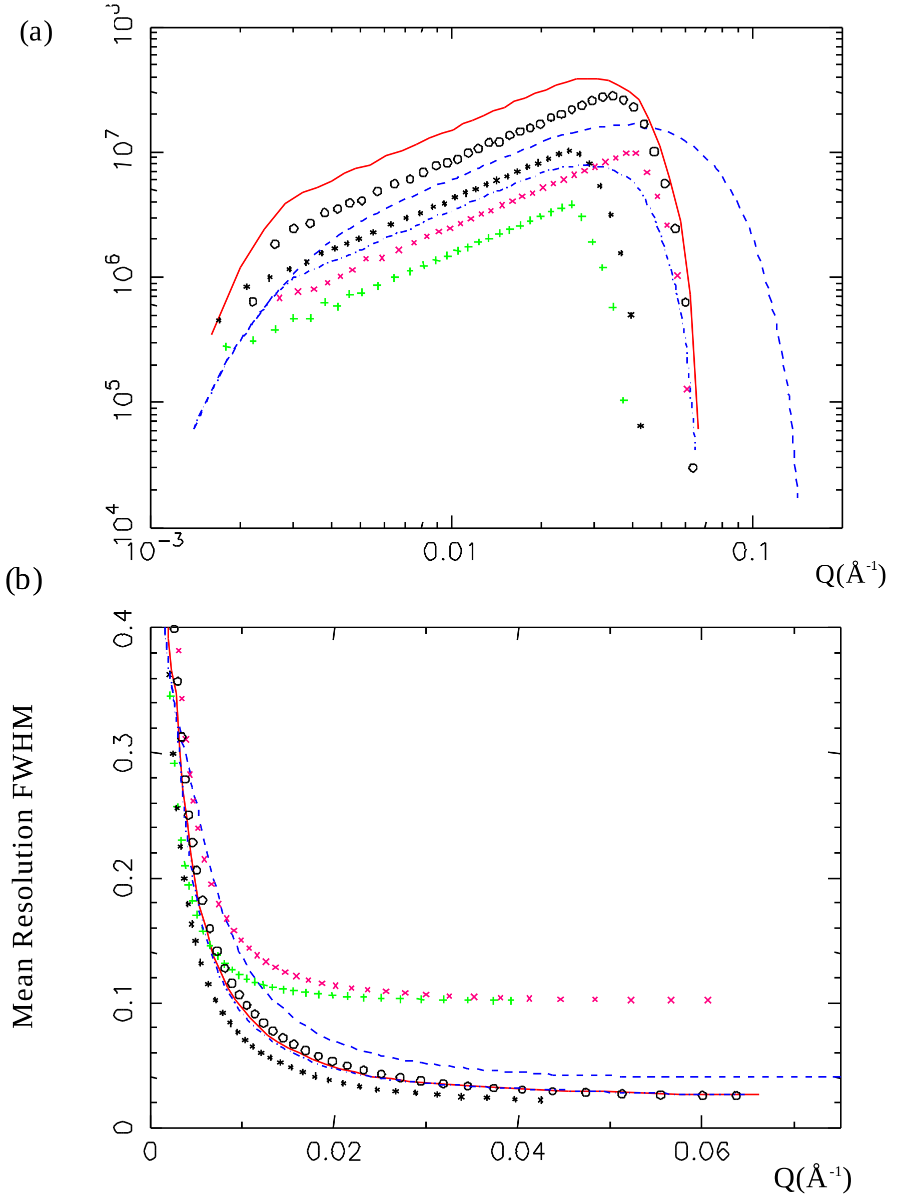

Fig.4: ESS - SANS At 36m (6/15/15), (a) $1cm^{-1}$ flat scatterer, (b) δQ/Q, FWHM resolution (Gaussian approximations) coupled H_2 moderator, 6mm diameter sample. Note changes to Q scales.

line - λ = 4.4 - 9.2 Å, 5MW, 16.6Hz, long pulse (Prompt spike at λ = 6.6 - 7.0 Å is still included here. Inelastic scatter from hydrogenous samples, separated by time-of-flight, reduces λ range from 4.4 to 11 down to say 4.4 - 9.2 or 7.5 - 11.0 Å),
circles -λ = 4.6 - 6.6 Å, 5MW, 50Hz
asterisk -λ = 6.8 - 8.8 Å, 5MW, 50Hz
dashes - λ = 2-11 Å, 1MW, 10Hz (full Q range truncated in (b)),
dot-dash - λ = 4.4-11 Å, 1MW, 10Hz (improve resolution by omitting short λ near beam stop)
xxx - λ = 5 Å, +++ - λ = 8 Å, 10% FWHM, ~"ILL reactor"

SANS at 50Hz, ~5MW

At 50Hz count rates are good but only on a smaller Q range, particularly at longer distances, due to smaller λ band pass. Thus this case is most similar to a reactor. Three choppers are required in the collimation section to remove frame overlap, as a single chopper would not be allowed close enough to the moderator.

Removing pulses to operate at 25Hz, 12.5Hz, 10Hz expands the Q range, but could leave prompt spike(s) in the frame (Fig. 2). Working at progressively lower repetition rates would ultimately give roughly the same Q range and count rates as the curves shown for 10Hz and 1MW, though some intermediate compromises could be attractive for many experiments.

The guide/bender section could be made shorter than indicated in Figures 3 and 4 to minimise the overall length of the beam line and improve Q ranges over those shown here. This is however done at the risk of higher backgrounds, and worse geometrical constraints with neighbouring beams.

Other more exotic solutions to expand the Q range are to rapidly re-phase choppers during runs or to use a system of choppers that simultaneously passes two λ bands over a 40msec collection frame.

SANS at 10Hz, ~1MW

The lowest repetition rate allows the largest λ band pass, as illustrated in Table 1, and gives the best simultaneous Q ranges (e.g. 0.0015 to > 0.1 $Å^{-1}$), using the significant flux from λ down to ~2 Å. The fall off in count rate at very low Q does not suit weak scatterers but is fine for stronger ones where the higher counts at middle Q provide good detail where the cross section is lower. Inclusion of shorter λ close to beam stop worsens Q resolution due to a 1/λ term, though these can easily be omitted in the final data reduction (as illustrated in Fig. 3b & 4b).

At the smallest Q, longest λ, a 5MW source at either 16.6Hz or 50Hz will always have more counts (Fig. 3 & 4). However even at 1MW there is potential to do better than the ILL over much of the Q range, particularly if the advantages of a wide simultaneous Q range are important. At 10Hz a single double disc chopper at L < 10m is sufficient to remove frame overlap. At longer L_2 and longer λ time of flight could be used to partially separate the 30-50% inelastic component of supposed incoherent background from H_2O etc. thus improving signal/background for dilute samples.

Further opportunities for SANS.

(i) At longer L_2 and longer λ time of flight could be used to largely separate the 30-50% inelastic component of supposed incoherent background from H_2O etc., leaving a nearly pure coherent signal thus improving signal/background for weak scatterers. With a sample at 21m and detector at 36m suitable wavelength bands for which this might be achieved are for example: 4.0 - 4.5 Å (on a short pulse source), 6.0 - 7.0 Å, 7.5 - 9.0 Å or 8.3 - 10.0 Å. Some reduction of repetition rate is also required, so count rates would be relatively low.

(ii) Further opportunities might be afforded using focussing mirror technologies currently under development to give improved count rates at very small Q with a relatively short beam line (Alefeld et.al.). The neutron beam is focussed at the detector to produce a two dimensional scattering pattern which is more useful and more appropriate for a white beam instrument than the slit smeared pattern from the Bonse-Hart, double crystal, method. To reach Q ~0.001 $Å^{-1}$ should be relatively simple, the goal of Q to ~ 10^{-4} $Å^{-1}$ is more technically challenging.

In summary

In all cases where inhomogeneities on different length scale are present the required Q range of 2-3 orders of magnitude can only be realised by repeated measurements at different sample to-detector distances. In such widely encountered cases the Q range accessib-le in a single shot (which is largest in the 10Hz) is no longer the most important criteria for the optimisation of the target station. Instead we would search for the target which gives the highest intensity for a certain Q-range where the resolution in Q should be roughly constant. Comparing the results of Fig. 3 and 4 the overall intensities at the same distance is by a factor of 3 - 4 times better for the 16.6Hz long pulse solution. Careful compromise of instrument design gives Q resolution approaching that of a short pulse target and still better than on a reactor.

The very best Q resolution (e.g. for diblock copolymers at low Q or liquid crystals at higher Q) is still however achieved on a short pulse target, selecting an appropriate wavelength band. Therefore a separate SANS instrument optimised for best Q resolution should be installed at the 50Hz, short pulse target station.

In other cases such as studies of anisotropic systems or ones changing in real time a wide simultaneous Q range is a distinct advantage of a pulsed source. Though 10Hz provides the best situation operation at sub-multiples of a 16.6Hz or 50Hz source frequency will be attractive for many experiments despite some issues of background signals.

Development and use of still larger area detectors is highly recommended in order to increase the simultaneously accessible Q range and count rate.

The combination of two instruments, one for lower wavelength resolution at a long-pulse 16.6Hz target station for main applications in conventional SANS and a second one (with the sample perhaps closer to the moderator) for high wavelength resolution at the 50Hz target would provide a world - leading experimental suite for SANS.