

# Indirect Geometry Spectrometers

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We looked at six instruments, covering a very wide range of science and energy scales:

- Backscattering
  - 0.8  $\mu\text{eV}$  – direct-backscattering Si 111
  - 1.5  $\mu\text{eV}$  – near-backscattering Si 111
  - 17  $\mu\text{eV}$  – near-backscattering PG 002
- Constant-**Q** (PRISMA)
- Vibrational Spectroscopy (TOSCA)
- Resonance High-Energy (eV spectroscopy)

The backscattering instruments cover quasielastic and inelastic measurements over a range of resolutions. The use of pulse-shaping choppers is considered in some detail, assuming that the pulse-shaping chopper needs to be outside the bulk shielding of the target station. The resultant loss of dynamic range is found to be unimportant for the Si ( $\sim 1 \mu\text{eV}$ ) machines, but very significant for the 17  $\mu\text{eV}$  (graphite) machine. The 0.8  $\mu\text{eV}$  machine is best served by a cold coupled moderator with a pulse-shaping chopper on the 50Hz target. This combination is also optimal for the 1.5  $\mu\text{eV}$  machine. Though the cold poisoned moderator without pulse-shaping performs just as well for quasielastic measurements, the use of a coupled moderator and a pulse-shaping chopper allows a more flexible tuning of the resolution, particularly for inelastic measurements. The graphite machine can be served by a range of moderators, giving different combinations of flux and dynamic range. The best option is probably the decoupled cold moderator on the 50Hz target. The Si machines outperform present reactor-based instruments by at least an order of magnitude in both flux and dynamic range simultaneously. The graphite machine outperforms IRIS by a factor of 200.

The constant-**Q** machine offers to cover a large fraction of experiments presently performed on triple-axis instruments. It uses an array of analyser arms to construct an energy scan at constant **Q** from a single measurement. The preferred moderator is the decoupled hydrogen moderator on the 50Hz target. Evaluation of the instrument is not sufficiently advanced to make quantitative comparisons with existing instruments.

The vibrational spectroscopy instrument is very similar to the present TOSCA instrument at ISIS. It measures the vibrational density of states over a wide range of energy transfers in a single measurement. The preferred moderator is decoupled hydrogen or poisoned water. The improvement in the source flux between ISIS and ESS is the major gain factor over TOSCA.

The eV spectroscopy instrument measures atomic momentum distributions by neutron Compton scattering. This instrument requires a poisoned moderator; thermal or cold on the 50Hz target.

Given the choice between the three proposed ESS targets, all six instruments identify the 50Hz short-pulse target as their first choice. 2 instruments choose the 10Hz short-pulse target as the second option. 2 instruments choose the long-pulse target as the second option.

## Backscattering Instruments

Three such instruments are examined.

- 1) 0.8  $\mu\text{eV}$  direct-backscattering machine using Si 111. Optimised for the best combination of resolution and counting rate for quasielastic measurements.
- 1) 1.5  $\mu\text{eV}$  near-backscattering machine using Si 111. Optimised for the best combination of resolution and counting rate inelastic measurements.
- 1) 17  $\mu\text{eV}$  near-backscattering machine using PG 002.

The 0.8  $\mu\text{eV}$  machine uses Si crystals arranged in direct backscattering (DBS) which means that the detectors are placed directly behind the sample (seen from the analysers). The secondary spectrometer resolution of this machine could be improved to 0.3-0.4  $\mu\text{eV}$  by using polished Si crystals and/or long secondary flight paths (3m or more). This instrument uses unpolished Si crystals at a distance of 2m from the sample to give a compact machine with a high counting rate and a resolution function without Lorentzian tails. It is optimised for quasielastic measurements, as performed at present on instruments such as IN16 and HFBS at NIST.

The 1.5  $\mu\text{eV}$  machine also uses unpolished Si crystals at 2m, but the detectors are arranged in near-backscattering (NBS), i.e. around and below the sample, so that direct line-of-sight from the sample to the detectors is eliminated. The penalty is a degradation in resolution, compared to DBS, but an improvement in background and potential "spurious". In a DBS instrument, elastic and quasielastic scattering from the sample directly into the detectors is eliminated using a "timing chopper". However, sharp inelastic events may still contaminate the data. NBS is thus a good choice for a truly inelastic machine.

The 17  $\mu\text{eV}$  machine uses pyrolytic graphite (PG) crystals in near-backscattering, at a distance of 1m from the sample, and cooled to about 10 K to reduce thermal diffuse scattering. It is very similar to IRIS at ISIS.

The DBS Si machine has a secondary spectrometer resolution of 0.56  $\mu\text{eV}$  FWHM. A timing chopper is used to discriminate against neutrons scattering directly into the detectors from the sample. This has the net effect of reducing the flux on the sample by a factor of two, which is taken into account in the flux numbers given here. The NBS Si machine has a secondary spectrometer resolution of 1.06  $\mu\text{eV}$  FWHM and no timing chopper. The graphite machine has a secondary spectrometer resolution of 12  $\mu\text{eV}$ . The secondary spectrometer resolution line shape is Gaussian for all three instruments.

The instruments are optimised to match the primary and secondary instrumental energy resolutions, i.e. the DBS Si machine is optimised for a total energy resolution of  $\sqrt{2} \times 0.56 \mu\text{eV} = 0.80 \mu\text{eV}$  and the NBS Si and graphite instruments have a total resolution of 1.50  $\mu\text{eV}$  and 17.0  $\mu\text{eV}$ , respectively. The resolution calculation includes the time-width from the moderator speed distribution, time-width (if applicable) from a

***The 0.8  $\mu\text{eV}$  Si backscattering instrument covers quasielastic measurements, in the same way as present-day reactor-based backscattering instruments.***

***The 1.5  $\mu\text{eV}$  Si instrument covers inelastic measurements.***

***The graphite instrument provides a resolution of 17  $\mu\text{eV}$  for both quasielastic and inelastic measurements.***

***The instruments are optimised by matching the primary and secondary resolution.***

pulse-shaping chopper, path-length uncertainty due to guide geometry and sample size. The resolution contributions are modelled as realistically as possible: The moderator shape is from the parameterisation circulated by the moderator working group. The pulse-shaping chopper contribution (if applicable) is triangular and the path-length uncertainties in the guide are calculated by Monte Carlo. The flux is calculated by numerical integration over the sampled region of the moderator time-speed distribution, combined with a Monte Carlo calculation of the guide transmission. The guide is straight with a cross-section of 60mm x70mm (W×H) and  $m=2$  supermirror coating. At the end, an  $m=4$  supermirror converging guide focuses the beam down to a sample size of 20mm x30mm (cylindrical). No systematic optimisation of the guide geometry has been performed. Increased gain factors can be obtained by using ballistic guides and improved-reflectivity supermirrors.

Instruments without pulse-shaping choppers rely on the intrinsic time-width of the moderator neutron distribution to give the desired energy resolution. Resolution is improved by moving away from the moderator. The table below summarises the essential instrument parameters for such instruments.

**Resolution and flux are calculated by a combination of numerical integration and Monte Carlo.**

**Conventional backscattering instruments: no pulse-shaping choppers.**

mod	$\Delta t$ ns	$L_i$ m	$\hbar\omega$ range 50Hz / 10Hz meV	$F(I_0)$ 50Hz / 10Hz $10^7$ n/cm <sup>2</sup> /s/Å
0.8 $\mu$ eV DBS Si machine				
1	27	235	-0.01 → 0.19 / 0.14	0.8 / 0.2
2	43	335	-0.01 → 0.14 / 0.86	1.6 / 0.3
4	59	440	-0.01 → 0.09 / 0.61	8.0 / 1.6
5	95	680	-0.01 → 0.06 / 0.36	15.6 / 3.1
1.5 $\mu$ eV NBS Si machine				
1	27	108	-0.01 → 0.47 / 6.05	1.8 / 0.4
2	43	155	-0.01 → 0.31 / 2.76	3.5 / 0.7
4	59	205	-0.01 → 0.23 / 1.73	16.8 / 3.4
5	95	315	-0.01 → 0.15 / 0.94	31.8 / 6.5
17 $\mu$ eV graphite machine				
4	60	14.4	-0.39 → 7.97 / -1.70 → 7.97	17 / 3
5	96	22.4	-0.10 → 3.53 / -1.57 → 6.97	33 / 7
6	229	71	-0.10 → 0.50 / -0.55 → 5.87	111 / 23

**Flux and dynamic range of conventional backscattering instruments:**

**0.8 meV machines are unfeasibly long.**

**1.5 meV machines are just about feasible**

**17 meV machines can be served by a range of moderators**

The moderator numbers refer to those specified by the moderator working group (1-3 thermal, 4-6 cold). The value of  $\Delta t$  given in the table is the FWHM of the moderator time-distribution at the elastic wavelength  $\lambda_0$  (6.27 Å for Si 111 and 6.70 Å for PG 002).  $L_i$  is the moderator-sample distance.  $\hbar\omega$  range is the useable range of energy transfers which is determined by a combination of repetition rate, instrument length, contamination from the first higher order reflection (Si 333 or PG 004, respectively), sweep time over the guide of the bandwidth (frame-overlap) chopper running at the source frequency and the requirement that the elastic peak must be included. The last column shows the time-averaged flux at the elastic wavelength.

Some of the flight paths for the Si instruments are very long

**The dynamic range is given by the need to eliminate frame overlap and higher-order contamination**

and probably unfeasible. In principle, there is no technical problem in building very long guides; the limiting factor is the cost. The cost of  $m=2$  supermirror guides is approx. 10 k\$/m for a typical guide cross-section, giving a price tag of 2 M\$ for a 200m guide. If we set the feasibility limit at around 200m, that leaves perhaps one instrument for the DBS Si instrument and three instruments for the NBS Si instruments.

Pulse-shaping choppers offer the possibility of improving resolution in a more flexible way than simply lengthening the instrument. A fast chopper is placed as close as possible to a coupled moderator. In principle, the enhanced peak flux from the coupled moderator can be combined with a much narrower time structure, given by the chopper speed. In practice, fast choppers cannot be placed arbitrarily close to the moderator for safety and maintenance reasons. Moving the pulse-shaping chopper away from the moderator translates into a reduced dynamic range. In these calculations, the pulse-shaping chopper is placed at a distance  $L_{\text{chop}}$  of 6.3 m from the moderator, which is the closest that can presently be achieved at ISIS. Either a Fermi or disk chopper can be used. At present the shortest burst time achievable with a disk chopper is about 15  $\mu\text{s}$  (FWHM) using a narrowed guide at the chopper position (NEAT, HMI). A Fermi chopper can achieve pulses as narrow as 2  $\mu\text{s}$  (ISIS). In these calculations, a triangular transmission function is used with a peak transmission of 100% without reference to the type of chopper. The table below gives  $\Delta t$  as the FWHM of this peak. To maximise the flux, the instrument length and chopper burst time are scanned together keeping the total resolution constant (at 0.8, 1.5 or 17  $\mu\text{eV}$ ). For the Si instruments, the flux on the sample was found to increase with instrument length beyond feasibility. We use 200m as the longest feasible guide length. This also coincides roughly with the length at which the dynamic range given by the instrument at 50 Hz matches the dynamic range given by the moderator-chopper distance. For the graphite machine, the length given in the table below corresponds to that of maximum flux at the elastic wavelength.

**Instruments much longer than 200 m are classed as unfeasible.**

**Pulse-shaping: a fast chopper close to the moderator defines the time-width of the pulse.**

**Placing the pulse-shaping chopper outside the bulk shielding significantly reduces the dynamic range.**

**Flux is maximised by scanning instrument length and chopper burst time together at constant resolution.**

**200 m is kept as the maximum feasible length.**

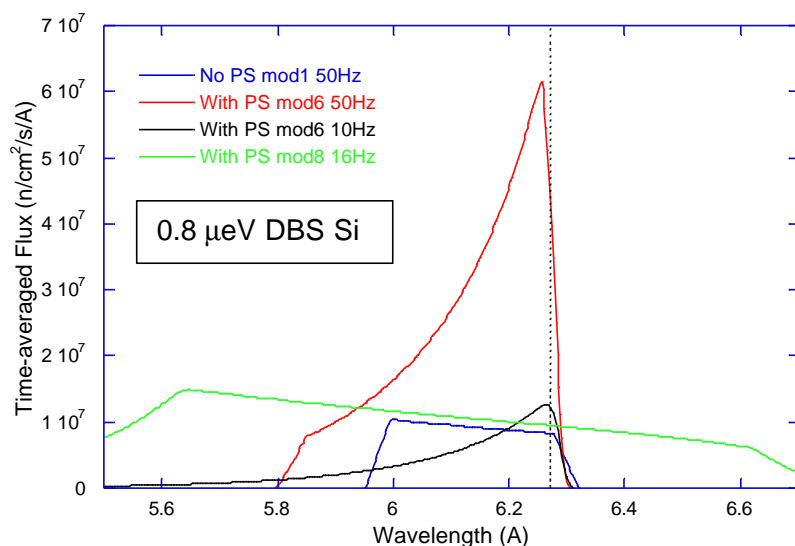
mod	f Hz	Dt ns	$L_i$ m	$\hbar w$ range meV	$F(I_0)$ $10^7 \text{ n/cm}^2/\text{s}/\text{\AA}$
0.8 $\mu\text{eV}$ DBS Si machine					
6	50	32	200	-0.02 $\rightarrow$ 0.27	6.2
6	10	32	200	-0.02 $\rightarrow$ 0.35	1.3
8	16	31	200	-0.21 $\rightarrow$ 0.73	1.0
1.5 $\mu\text{eV}$ NBS Si machine					
6	50	76	200	-0.05 $\rightarrow$ 0.23	27.5
6	10	76	200	-0.05 $\rightarrow$ 0.34	5.4
8	16	73	200	-0.21 $\rightarrow$ 0.73	4.4
17 $\mu\text{eV}$ graphite machine					
6	50	300	59.5	-0.15 $\rightarrow$ 0.26	50
6	10	300	59.5	-0.15 $\rightarrow$ 0.26	10
8	16	600	114	-0.30 $\rightarrow$ 0.88	32

**Flux and dynamic range of backscattering instruments with a pulse-shaping chopper**

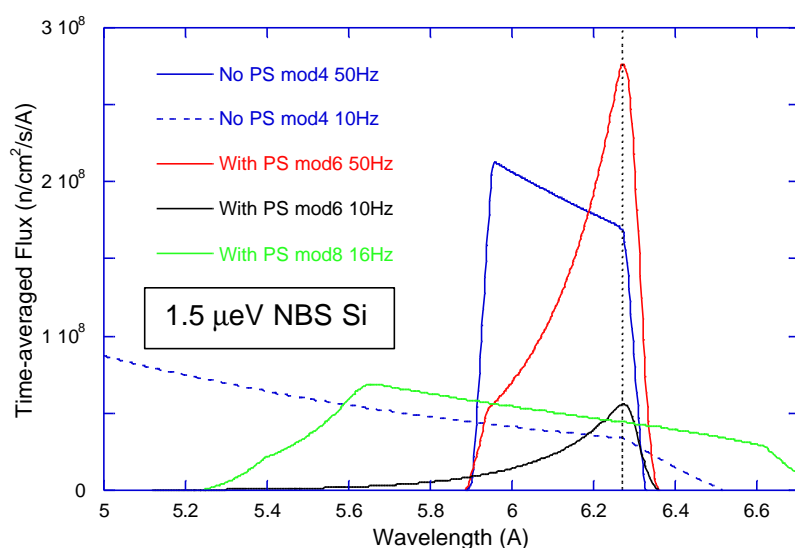
**0.8 and 1.5  $\mu\text{eV}$  instruments are 200 m long.**

**Long-pulse instruments have twice the dynamic range**

**17  $\mu\text{eV}$  instruments are shorter but with the same dynamic range.**



**The 0.8  $\mu\text{eV}$  instrument is best served using a pulse-shaping chopper.**



**The 1.5  $\mu\text{eV}$  instrument does equally well with and without a pulse-shaping chopper.**

**Fig. 1:** Flux versus wavelength for the Si backscattering machines. The elastic wavelength is indicated by the black dotted line. PS stands for pulse-shaping.

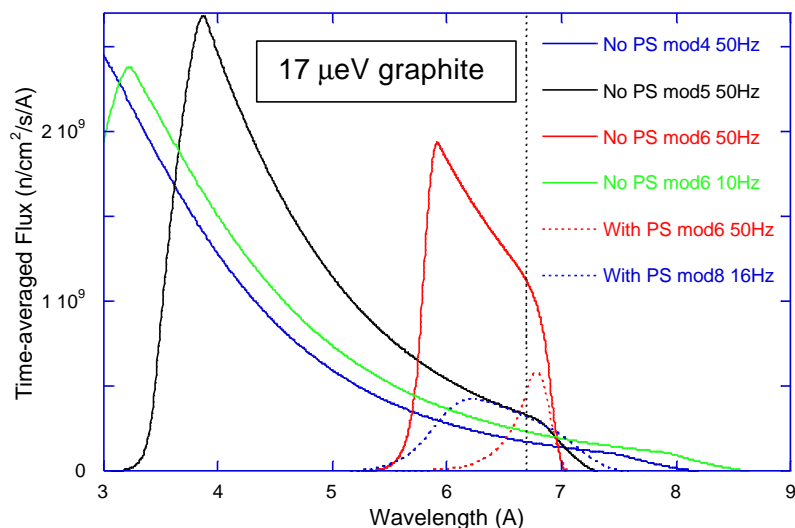
The highest flux on the 0.8  $\mu\text{eV}$  DBS instrument is achieved using a pulse-shaping (PS) chopper on the coupled cold moderator (mod6) at 50Hz. For the 1.5  $\mu\text{eV}$  NBS instrument, the 205m long conventional (no PS) instrument viewing the poisoned cold moderator (4) has a similar flux to the pulse-shaping instrument on the coupled moderator. The preference is for the pulse-shaping instrument, as it gives the flexibility to more closely match primary and secondary resolutions when measuring at large energy transfers. It also allows the option of increasing the flux by relaxing the resolution. For example, at an energy transfer of 10 meV, the conventional machine has a non-tuneable resolution of 6.3  $\mu\text{eV}$ , while the pulse-shaping machine can be tuned to give a resolution of between 3 and about 30  $\mu\text{eV}$ , with approximately the same flux at the same resolution. For both Si machines, the flux can be increased by about an order of magnitude by relaxing the resolution by an order of magnitude. There is also a small advantage for the long-pulse target: The long-pulse instruments can gain about twice as much flux as the instruments on the short-pulse target by relaxing resolution.

**For the Si machines, a pulse-shaping chopper is the best option: it provides far higher flux for the 0.8  $\mu\text{eV}$  machine and tuneable resolution for both machines.**

**For the 1.5  $\mu\text{eV}$  machine, this means that primary and secondary resolutions can be more closely matched when measuring at large energy transfers.**

The dynamic range of the pulse-shaping instruments is up to three orders of magnitude greater than the resolution width and is thus more than adequate for quasielastic scattering and also for inelastic measurements after a survey measurement has been done elsewhere. For both instruments, the long-pulse target offers an increase in dynamic range by about a factor of two with a decrease in flux by a factor of 2-3. The 10Hz target is of no interest, combining the reduced dynamic range of the 50Hz pulse-shaping machines with the reduced flux of the long-pulse target.

**The 50Hz target offers the highest flux with a good dynamic range. The long-pulse target provides twice the dynamic range with half the flux. The 10Hz target is not competitive.**



**Fig. 2.** Flux versus wavelength for the graphite backscattering machine. The elastic wavelength is indicated by the black dotted line. PS stands for pulse-shaping.

**For the graphite instrument, pulse-shaping choppers are not competitive with conventional machines.**

A wide range of combinations of flux and dynamic range is available for the graphite machine. The conventional decoupled-moderator (mod5) instrument on the 50 Hz target (shown in black) gives a high flux with a dynamic range of 3.5 meV, representing a conventional compromise between flux and dynamic range. This is the reference graphite instrument, similar to IRIS at ISIS. The dynamic range of the pulse-shaping instruments (shown as dotted lines) is seen to be drastically reduced compared to the conventional instruments; down to about 0.4 meV with a similar flux as the reference instrument. The long-pulse instrument also has the same flux as the reference instrument at the elastic wavelength and a dynamic range of about 1 meV. Both pulse-shaping instruments are clearly uncompetitive compared to the 50Hz coupled-moderator instrument without pulse-shaping (shown in red) which provides a much higher flux at the elastic wavelength and a similar dynamic range.

**A wide range of combination of flux and dynamic range is available for conventional graphite machines.**

**The reference graphite instrument views the decoupled hydrogen moderator.**

The flux on the graphite pulse-shaping instruments cannot be increased much by relaxing resolution, as the opening time of the pulse-shaping chopper is already comparable to the intrinsic moderator time width. On the short-pulse target, there is no flux gain to be made, while on the long-pulse target the flux can be increased by about a factor of two by relaxing the resolution by a factor of two.

**On the pulse-shaping graphite instruments, only marginal flux increases can be gained by relaxing resolution.**

We compare the performance of the Si instruments with IN16 at the ILL and the High Flux Backscattering Spectrometer (HFBS) at NIST.

The energy resolution on IN16 is 0.9  $\mu\text{eV}$  (FWHM) giving a flux on the sample of  $1 \times 10^5 \text{ n/cm}^2/\text{s}$  over a dynamic range of  $-15 \rightarrow 15 \mu\text{eV}$ . The best energy resolution on HFBS is 0.80  $\mu\text{eV}$  (FWHM) giving a flux on the sample of  $1.4 \times 10^5 \text{ n/cm}^2/\text{s}$  over a dynamic range of  $-11 \rightarrow 11 \mu\text{eV}$ . Integrating over the corresponding wavelength ranges for the ESS 50Hz coupled-moderator instrument with pulse-shaping, gives a flux of  $2.5 \times 10^6 \text{ n/cm}^2/\text{s}$  and  $2 \times 10^6 \text{ n/cm}^2/\text{s}$ , respectively, for these two dynamic ranges. The flux is 25 times higher than IN16 and 14 times higher than HFBS. In addition, for both these instruments, the dynamic range of the ESS instrument is an order of magnitude greater.

***The 0.8 meV instrument has 20 times higher flux at the elastic wavelength than the present best (HFBS and IN16) and an order of magnitude greater dynamic range.***

Comparing with the 1.5  $\mu\text{eV}$  instrument is not as straightforward, as there is no truly inelastic instrument of this type in existence. For a flux comparison, we use the broadest energy resolution available on HFBS, which is 1.01  $\mu\text{eV}$  (FWHM) giving a flux on the sample of  $1.4 \times 10^5 \text{ n/cm}^2/\text{s}$  over a dynamic range of  $-36 \rightarrow 36 \mu\text{eV}$ . Integrating over the corresponding wavelength range for the ESS 50Hz coupled-moderator instrument with pulse-shaping, gives a flux of  $2.5 \times 10^7 \text{ n/cm}^2/\text{s}$ , which is more than 2 orders of magnitude higher. The resolution of the ESS instrument is about 50% broader, while the dynamic range is an order of magnitude greater.

***The 1.5 meV instrument has more than 100 times higher flux than the closest existing instrument.***

The two existing instruments in Europe which come closest to the graphite machine are IRIS at ISIS and IN13 at the ILL. IN13 has an energy resolution of 8  $\mu\text{eV}$  and a dynamic range from  $-0.12$  to 0.3 meV. It has a Q-range about twice as wide as this instrument. The monochromatic flux on IN13 is  $2 \times 10^4 \text{ n/cm}^2/\text{s}$ . The ESS 50Hz reference instrument is calculated to give a flux of  $33 \times 10^7 \text{ n/cm}^2/\text{s}/\text{\AA}$  at  $\lambda = 6.7 \text{ \AA}$ . Integrating over the resolution width ( $\Delta E = 0.017 \text{ meV}$  gives  $\Delta \lambda = 0.031 \text{ \AA}$ ) gives a "monochromatic" flux of  $1.0 \times 10^7 \text{ n/cm}^2/\text{s}$ , nearly three orders of magnitude higher than IN13.

***The graphite instrument has 500 times higher flux than IN13 and 150 times higher flux than IRIS.***

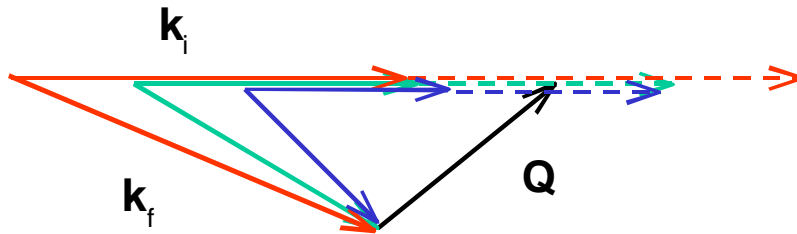
IRIS is very similar to the reference graphite instrument. It has an energy resolution of 17.5  $\mu\text{eV}$  using cooled PG 002 crystals and sits at a distance of 36.5m from the ISIS decoupled  $\text{H}_2$  moderator which has a similar time-structure to the ESS decoupled  $\text{H}_2$  moderator (for  $\lambda = 6.7 \text{ \AA}$ , ISIS  $\Delta t = 110 \mu\text{s}$  and ESS  $\Delta t = 96 \mu\text{s}$ ). The measured white beam flux on IRIS is  $5.0 \times 10^7 \text{ n/cm}^2/\text{s}$ . This translates into a flux of about  $1.3 \times 10^7 \text{ n/cm}^2/\text{s}$  for the integrated wavelength range from 4.6  $\text{ \AA}$  to 6.9  $\text{ \AA}$ . Over the same wavelength range, the ESS instrument gives a flux of  $1.8 \times 10^9 \text{ n/cm}^2/\text{s}$ , more than two orders of magnitude higher. This is to be expected as the instruments are basically identical except for the source which gives a factor of 30 increase in flux and the supermirror guide which can give another factor of 4 compared to the IRIS nickel guide.

## Constant-Q Instrument

Energy scans at constant wave vector  $\mathbf{Q}$  in a single crystal can be obtained in a single measurement using an indirect

***A multi-analyser-arm instrument can perform a***

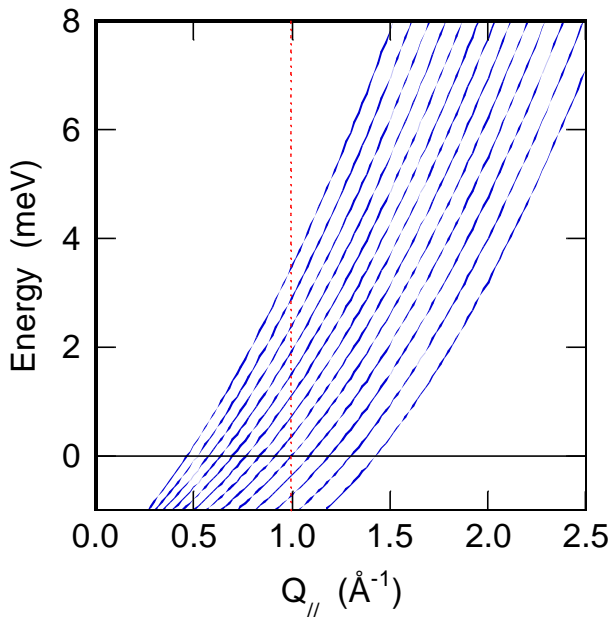
geometry spectrometer with a multianalyser array, where analyser arms at different scattering angles have different final energies. Each detector scans the energy along the direction of the incoming wave vector, i.e. along  $Q_{\parallel}$ . Each arm can be made to have the same  $Q_{\perp}$ , by adjusting  $k_f$  to the scattering angle  $\phi$  according to  $k_f = Q_{\perp}/\sin\phi$ , as illustrated:



**large fraction of triple-axis-type measurements.**

**The analysing energy of each arm is set so that a scan at constant  $Q$  can be constructed from a single measurement.**

By rebinning the detectors, a series of constant  $Q$  scans for different  $Q_{\parallel}$  and the same  $Q_{\perp}$  is then obtained:



A prototype spectrometer (PRISMA) has been in routine operation at ISIS for several years.

In order to be competitive with respect to triple-axis spectrometers and direct geometry chopper spectrometers, the energy resolution and dynamical range should match those types of spectrometers. The only suitable option seems to be to use the (002) reflection of pyrolytic graphite analysers, which gives an upper limit of the final energy of approximately 32 meV (due to space restrictions and deteriorating resolution), while the lowest useful final energy for measuring dispersive excitations in single crystals is approximately 2 meV. To avoid collisions between analyser arms, either a RITA-type arrangement of analysers and a position-sensitive detector or a vertical scattering geometry on the analyser side are envisaged.

In order to construct a reasonable constant- $Q$  scan without scanning the analyser angles, it is estimated that at least 20 analyser arms are needed with at most  $1^\circ$  separation.

This is a new type of instrument, which offers the exciting possibility of covering a large fraction of TAS-type measurements at a pulsed source. The resolution and flux are

**Graphite crystals are used for energy analysis and the most promising scattering geometry for the analysers may well be vertical.**

**At least 20 analyser arms are needed with at most  $1^\circ$  separation.**

**The resolution is less tuneable than on a triple-**



significantly less tuneable, as they are largely dictated by non-adjustable parameters, such as the position in  $(\mathbf{Q}, \omega)$ -space being measured and to a lesser extent, the moderator characteristics and instrument length.

The highest useful incident energy is limited to four times the final energy by second-order reflections of the analysers. This defines the dynamical range of the spectrometer. The energy resolution for *elastic* energy transfer can be approximated as

$$\Delta E / E = 2\sqrt{(\Delta t/t)^2 + (\cot \mathbf{q} \Delta \mathbf{q})^2} \quad (1)$$

where  $\Delta \theta$  will be of the order of one degree, as collimators should be avoided due to space restrictions. In order to be competitive with a TAS equipped with collimators, the  $\Delta t/t$  term is only allowed to increase the total  $\Delta E/E$  by 10-20%. This has the auxiliary advantage of giving a nearly Gaussian resolution function, important for line shape analysis. For elastic scattering, the restriction on  $\Delta t$  given by Eq. (1) is only important at low final energies, where the  $\Delta \theta$  term is small. However, as the energy transfer increases, the term  $\Delta t/t$  increases in importance. For a final energy of 2 meV, we find from Eq. (1) that the longest acceptable  $\Delta t$  (in microseconds) for elastic scattering is

$$\Delta t = 5.1 L_i \quad (2)$$

where  $L_i$  is the incident flight path (in meters). As usual, longer pulse widths can be accepted by increasing the length of the primary spectrometer.

Due to frame overlap, the length of the primary spectrometer is limited by the pulse repetition rate. For a final energy of 2 meV (the limiting case), allowing for a large dynamical range, the longest distances will be approximately 12, 25, 38, and 63 m, for pulse repetition rates of 50, 25, 16.7, and 10Hz, respectively.

We have calculated the time-averaged flux at the sample position for these four different distances using the moderators that can fulfil the resolution requirement Eq. (2). A straight  $m=3$  supermirror guide starting at 1.7m from the moderator surface is included. The last 4m consists of an  $m=4$  focusing supermirror guide. At the low-energy end, the best solution appears to be a 17Hz 38m source with a coupled liquid hydrogen moderator (6) while the high-energy end is better served by a 25Hz 25m source, with a coupled ambient water moderator. Since the energy resolution due to the crystal analyzers deteriorates rapidly with increasing final energy, it appears best to optimize the spectrometer for cold neutrons. Given the choice between 10Hz and 50Hz target stations, the preference for this instrument is for the 50Hz target station with a decoupled hydrogen moderator. The long-pulse option with a pulse-shaping chopper at 6.3m and an instrument length of 160m using a coupled liquid hydrogen moderator is also interesting concerning flux, but the band width is reduced to only 1.2 Å. The flux gain would then in many cases be outweighed by the increase in measuring time, as several measurements using different incident energy ranges are required. The full optimization for strongly inelastic scattering remains to be done.

***axis instrument.***

***Liquid H<sub>2</sub> is probably the best option.***

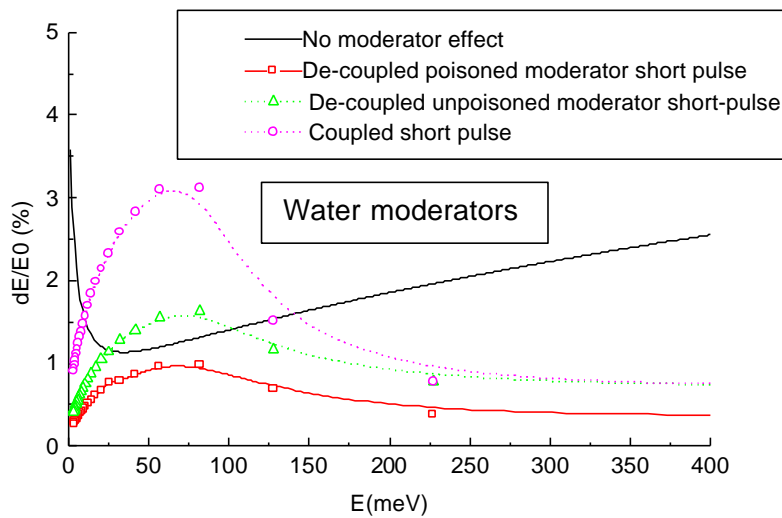
***The 50Hz target is preferred with the 10Hz target as the second option.***

***The long-pulse target is probably not useful.***

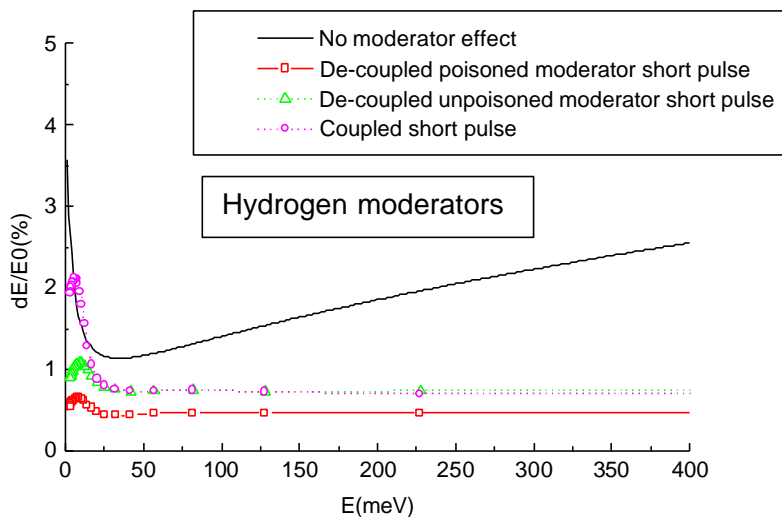
## Vibrational Spectroscopy Spectrometer

This is an instrument specialised for the measurement of the vibrational density of states, very similar to the TOSCA spectrometer at ISIS. It uses graphite 002 analysers with a fixed take-off angle, covering as large a fraction of the available solid angle as possible. Cooled Be filters are used to eliminate higher-order contamination. The instrument needs to cover a range of energy transfers from 0 to 1000 meV in a single measurement, which corresponds to a wavelength range of 0.2 to 5.0 Å. The two figures below show the instrumental energy resolution for the water and hydrogen moderators respectively.

***An instrument for measuring the vibrational density of states, similar to Raman and infrared light scattering.***



***Of the water moderators, only the poisoned moderator can match the secondary spectrometer resolution.***



***The decoupled hydrogen moderator can do even better.***

The solid line shows the secondary spectrometer resolution for a TOSCA-type instrument. From these figures, the best moderators are poisoned water and decoupled hydrogen, with the decoupled hydrogen moderator giving an increased flux at longer wavelengths. The long-pulse target cannot be used, as without pulse-shaping the resolution is too poor and with pulse-shaping the dynamic range is too restricted.

***The preferred moderators are the poisoned water and decoupled hydrogen.***

***The long-pulse target is ruled out.***

For this type of instrument, the 50Hz target offers the highest flux. The 10Hz target is also of interest for a longer, high-resolution version with the same dynamic range.

**The preferred target station is 50Hz with the 10Hz target as an interesting second option.**

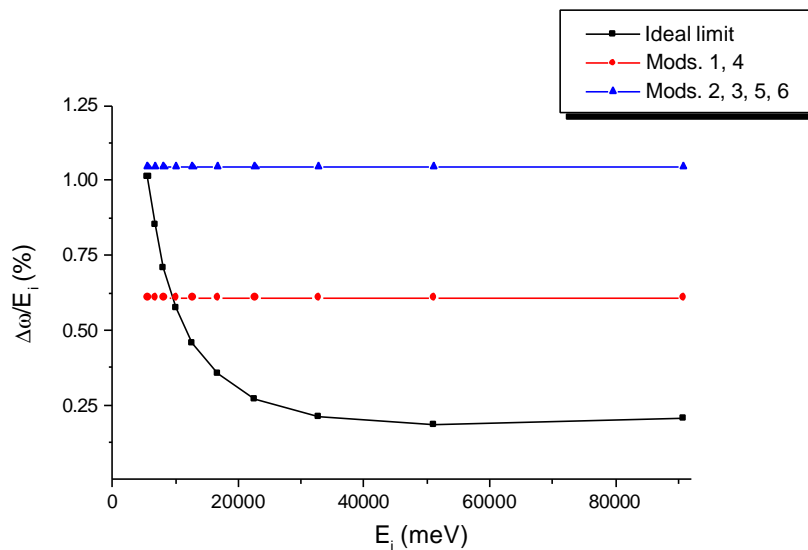
## Resonance High-Energy Spectrometer

This instrument uses the resonant neutron absorption of  $^{238}\text{U}$  at 6.67 eV as energy analyser. It is similar to the eVS spectrometer at ISIS. Neutron Compton scattering is used to measure the momentum distribution, mainly of light atoms, e.g. H, D, He or C. The typical incoming energy range is 5 to 64 eV, corresponding to wavelengths between 0.04 and 0.11 Å, in the non-Maxwellian part of the neutron spectrum.

**Neutron Compton scattering: measuring atomic momentum distributions.**

**Very high energies: non-Maxwellian part of spectrum.**

The energy resolution for the different moderators is shown below:



**Far from Maxwellian => moderator temperature is unimportant**

**Coupling is unimportant**

**Only moderator size matters: poisoned moderator is best.**

The black line shows the secondary spectrometer resolution for a realistic instrument geometry. We can easily see that the choice of a suitable moderator is restricted to either number 1 or 4 only, if the machine has to be pushed close to its theoretical energy-resolution limit.

**The optimal moderator is poisoned water or hydrogen.**

To match the secondary spectrometer resolution, the time-width of the neutron pulse needs to be significantly less than 1 μs, which is not achievable with present-day choppers. This rules out the use of the long-pulse target.

The ideal repetition rate is of the order of 1kHz, which makes our choice of the 50Hz target an easy one.

**The 50Hz target station is preferred.**

