Instrumentation: report on the presentation and discussions

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Choice of Spectrometers

The instrumentation sessions began by presentations on the WNR, ZING P', IPNS-1, Harwell and KENS spectrometers which have been constructed, or at least fully designed. It was interesting to see how the different laboratories had followed rather different selections from the available instrument ideas. The table summarises these and other instrument portfolios.

		WNR	ZING P'	(IPNS-1)	Harwell	(Rutherford)	KENS	Tohoku
Total	Total scattering (>1%)	2			1	(1)	1	3
	Total scattering (<0.3%)		1	(2)	1	(1)		
	Total scattering (0.03%)					(1)		
	Small angle diffraction	(1)	1	1	1	(2)	1	
	Single crystal diffraction	1	1	(1)	1	(1)	(1)	2
Inelastic	Direct geometry inelastic	1	1	(2)	1	(2)		1
	Incoherent inelastic	2	1	1	(1)	(1)		1
	Incoherent quasielastic					(1)	1	
	Coherent inelastic				1	(2)	1	
Special	Active Sample				1			
	UCN		1	1				
	Polarised neutron				1		1+(1)	1
	Resonance detector	1			1			
	Epithermal diffractometer				1			

( ) means designed but not constructed.

Thus while total scattering is universally represented, there are interesting differences in emphasis. Liquid and amorphous structure factors can be measured with minimum (>1%) resolution. Powder refinements can be made at this resolution, but high order peaks overlap, so that much better refinements are possible at <0.3% resolution spectrometers.

Small angle scattering is being almost universally attempted because of its importance. On the whole however the table shows few cold neutron instruments. This is in keeping with the principle that pulsed neutron sources will compete best against steady sources for high energy incident neutron experiments.

Single crystal instruments are again universally being tried and, although single crystal measurements will usually be necessary for the solution of unknown structures, it is not yet clear how well these can compete for structural refinements against powder measurements. Intrinsically they are less efficient as much of each time-of-flight spectrum measures empty background. However the use of position sensitive detectors may well give them back the advantage.

While all centres are trying direct geometry spectrometers with a pulsed monochromatic beam, there is no consensus as to the best method. Most centres have chosen a double rotor design with the main thermal neutron chopper preceded by a fast neutron "stopper." However the Tohoku spectrometer uses a rotating crystal method, the Harwell spectrometer a combined function reactor-style fast neutron stopping rotor, and WNR plans to run without any fast neutron chopping at all with the philosophy of letting the fast neutrons go past the spectrometer.

The division of crystal analyser/beryllium filter spectrometers

into vibrational and diffusional spectrometers became apparent. Nearly all laboratories plan such spectrometers for high Q, high ω vibrational spectrometry. On the other hand LAM at KENS and IRIS at SNS are designed for quasi-elastic studies with long wavelength incident neutrons. From the point of view of machine design they must be quite different with the high energy transfer machines designed with good scattered flight time focussing and the quasi-elastic machines designed with good scattered energy resolution.

The coherent inelastic machines are all inverted geometry crystal analyser spectrometers. The two designs of the Constant Q Spectrometer using the MARX principle, and the High Symmetry Spectrometer using independent analyser crystals have been the only geometries yet tried.

Most laboratories have chosen their own selection of special purpose spectrometers, reflecting their special interests. The active sample diffractometer with its short L_0 and long L_1 has yet to be tested but has many applied research applications for nuclear laboratories. Ultra-cold neutrons (UCN) have certain advantages on pulsed sources. In particular, access to the "source" is easy, heat fluxes into the moderator are low, and the "turbine" method is naturally suited to pulsed sources. Polarised neutrons have also been linked to cold neutrons in the past, where magnetic supermirrors give easy and efficient polarisation. Their use on epithermal beams depends on the development of good white beam polarisers and this is reported on later. We saw no consensus of design on polarised neutron spectrometers.

It is not yet clear how far up in energy neutron scattering will extend in the future. The total-cross-section, resonance

detector, and epithermal diffractometer all have in common that they use >1000 meV incident energy neutrons. These spectrometers did not receive much attention at the meeting, although if background problems can be solved, these spectrometers allow perhaps our best opportunity to break into new fields of neutron scattering physics quite impossible on reactor sources.

Instrumentation on Long-Pulse Sources

We heard from our German colleagues, Alefeld, Bauer, and Nücker, many new ideas on instrumentation for their 500 μs pulselength 1/20 duty cycle SNQ source. Clearly there are many new instrument ideas waiting to be discovered or exploited in this field. We had one example each of the use of moving samples, multiple monochromators, correlation methods and polarisation control.

The suggestion of Price to pseudo-randomly pulse a semi-continuous source at a relatively fast speed commensurate with the moderation time at the wavelength of interest ($\sim 10 \lambda$ μs Å^{-1}), left echoes which reverberated throughout the week. Clearly such a source would give very high performance for all experiments which could exploit the correlation methods. These seem to include most of the important spectrometers. For example it was suggested in the summary presentation that time-of-flight diffraction would be particularly easy and effective on such a source as shown in figure A. The problem with the pseudo-random source is its optimisation for all wavelengths simultaneously. The SNQ is well suited to cold neutron generation, but in the case of say 6 Å neutrons the moderation time is $\sim$100 μs, so that optimum performance

is nearly attainable by reducing the total pulse length to around this value rather than by pseudo-random pulsing.

The use of the SNQ for coherent inelastic scattering was explored in private discussions. A possible method analogous to MAX is shown in figure B.

The SIN spectrometers were not presented as they will be so similar to existing reactor designs. The big uncertainty in many minds was how far it will be possible to shield the counters in the spectrometers from the fast neutron pulse as the proton beam fires. Existing experience on pulsed sources suggests that background neutrons within 100 μs of the time of fast neutron generation are not stopped by conventional spectrometer shielding (∿20 cm borated paraffin). However unconventional methods may bring a solution. For example it may be necessary for monochromator housings to have a "get lost" beam tube leading to a carefully designed beam dump which will moderate and absorb the fast neutrons at an area remote from the spectrometer itself.

Instrument Design

During the instrumentation sessions several interesting differences of design became apparent.

Liquids and Amorphous Diffractometers

Perhaps the most important was that of total scattering. Figure C shows the two extreme views.

(1) The conventional approach uses discrete counter banks each optimised to give the best performance at its own scattering angle. Usually there are massive high angle counter banks with full time focussing. At lower angles there are Debye-Scherrer ring collimators at each angle, and for small angles a separate longer flight path detector bank. Each bank is surrounded by a massive fast neutron shield.

(2) The new approach of IPNS-1 followed in some respects at WNR and KEK is to surround the sample with a "blanket" of counters at all angles. Each counter must then be electronically processed to give a cross-section $S(Q, \lambda)$. The background problem is tackled by the use of a large vacuum chamber. Experience at KENS with the diffractmeter HIT suggests that background can be kept tolerable in such a spectrometer at any rate above 0.5 Å.

Powder Diffractometers

In the case of powder spectroscopy it was clear that the back scattering banks are the crucial ones for giving precision in profile refinements. The SNS project powder spectrometers were described. They include a 0.03% resolution spectrometer incorperating a 100 m guide tube in the incident flight path with a very large flat back scattering position sensitive detector.

Small Angle Diffractometers

This important subject received much discussion inside and outside the sessions. There are several points of principle still not settled. For example, is a 22K source essential or can we work in the 1-4 Å range where ambiant or 77K moderators give good neutron fluxes? Do we need to shield our detector from fast neutrons or can we simply ignore the 500 μs after the fast neutron pulse?

The results from the prototype spectrometers at WNR and ZING P' were not presented in any detail. The KENS spectrometer results suggested that we cannot count through the fast neutron pulse, but that background was no problem in a cadmium shielded enclosure over the 500 to 20,000 μs time range. We heard from Stewart a most interesting discussion of the problems of combining data from different wavelength ranges. Because of the absorption, multiple scattering and various background corrections, there is very little point in trying to combine raw data from a wide range of wavelengths. A good fit of cross-sections from the full range can only emerge after full processing on a main frame computer. While the results from KENS looked very promising in that intense scattering was seen in minutes, we must await a full study before this important spectrometer can be added to the pulsed source portfolio.

Single crystal diffraction

We heard accounts of the ZING P', Tohoku and WNR Spectrometers. Tohoku uses a one-dimensional counter, the others much smaller two dimensional counters. In fact a wide angular range seems highly desirable if we are to achieve the objective of measuring each reflection as a function of wavelength. The real need is to assess the accuracy of the data quantitatively. Both ZING P' and Tohoku have studied NaCl with the object of obtaining a full data set. Both reported preliminary data but the data processing problems are large simply because of the vast amounts of data produced. An hours run produces perhaps 64 x 64 position x 512 time channels! The Tohoku group described an automated analysis procedure for locating peak centroids, in reciprocal space, evaluating their structure factor corrected for local background, and discriminating against

spurious peaks from noise fluctuations.

Direct Geometry Inelastic

For once there was a general conformity of design. Most discussion centred on the difficult problems of rotor phasing. It now seems generally realised that different energy ranges can be covered by just one spectrometer according to the value of the chopper pulse width. The incident flight path L_0 determines the overall resolution. The optimisation of L_1/L_0, the ratio of scattered to incident paths, was discussed. This can only be done for some assumed ratio of energies E_1/E_0. This leads naturally to the SNS designs when a larger L_1/L_0 is specified for low angles where $E_1 \sim E_0$, than for high angles when $E_1 \sim \frac{1}{2}E_0$ and a smaller $\frac{L_1}{L_0}$ is optimum.

Incoherent Inelastic

There are two quite different concepts for this type of measurement, as shown in figure D. In (i) a crystal analyser defines the k_1 value while k_0 is defined by time-of-flight. In (ii) a beryllium filter is used to select only neutrons with energies below the Bragg cut-off (0-5 meV). We thus select a "window" of scattered energies 5 meV wide and again determine E_0 from time-of-flight.

We saw from WNR the interesting comparison of results from the same sample at the same flightpath by the two methods. The analyser method gave of course the cleanest spectra but the filter method gave 100 times the intensity with only 10 times the background! In addition the filter method gave sharp "edges" on most peaks which define the peak energy essentially to as good an accuracy as the analyser method. Thus the question as to which method to use is

still wide open.

Coherent Inelastic

We saw early results from MAX and phonons and magrons from a single crystal of iron. It is clear that lining up the spectrometer with its 15 independent analysers is an important preliminary to obtaining accurate results. Methods using time-of-flight to determine angles directly with respect to their zero angles ($2\theta_s - 2\theta_s^{zero}$) and ($2\theta_A - 2\theta_A^{zero}$) will probably be most precise. The choice of scan in reciprocal space is crucial. Only around certain reciprocal lattice points will the scan around a given reduced $\underline{q}$ and $\hbar\omega$ be with an appropriate E_0 and ratio E_1/E_0 to give a "nice" scattering triangle. Higher order reflections from the analyser are certainly a problem. This is partly because if one order, say graphite (002), gives a high symmetry direction scan through the (111) reciprocal lattice pcint, the (004) gives a parallel scan through the (222) point. Thus there is an enhanced cpportunity for Bragg or low energy phonon scattering from the high orders. On the other hand the higher order scans are often well separated from the low order scan and offer an alternative set of measurements along the same symmetry direction.

Spectrometer Results

Liquid and Amorphous Structures

The many results from amorphous materials, shown by Suzuki, have already brought worldwide fame to Tohoku. An extension of the pulsed method to study transient structures was described by Shinohe. He presented structure factors from super-cooled and just

solidified materials. This type of measurement is highly suited to the pulsed source.

Powder Profile Refinement

Outstanding results were presented from ZING P'. The results of refinement of a beta" alumina, for example (see Borso et al.), show clearly that the pulsed method gives as good a fit as conventional reactor methods. The fact that the important high $\sin\theta/\lambda$ region is extended means that the spatial precision of structural and thermal parameters will in general be better than with reactor data. The 3 pages of experiment titles completed on the ZING P' spectrometer means that the method is now entering a routine stage.

Incoherent Inelastic

Data from the ZING P' spectrometer were presented on several hydride materials, organic materials and even biological samples. The hydride samples showed up to four harmonics---perhaps a record! Again a list of completed experiments convinced one that the spectrometer is fully established.

Quasielastic

Inoue's results from the LAMDA spectrometer at Hokkaido and LAM at KENS provided a welcome contrast as a fully developed spectrometer with an extensive list of important experiments completed. We saw the excellent capability of the spectrometer to measure diffusion constants in the water range and therefore to distinguish free and bound water.

The Use of Peak Fluxes

In the summary session Windsor presented a plea for restraint in the use of peak fluxes or equivalent reactor fluxes in contexts where they will be compared with reactor fluxes. The reason is partly that the true figure of merit for most experiments is

$$\frac{\text{(peak flux) x (moderator area) x (pulse repitition frequency)}}{\text{(pulse width)}}$$

Thus "hot" neutron performance is underestimated relative to cold neutron performance because of the change in pulse width. Perhaps of more importance is the fact illustrated below that while the pulsed flux shines directly onto one sample where it can be wavelength analysed by time-of-flight, the reactor source must be monochromated (or chopped) before it is useful. Thus the comparison depends on the detailed performance of crystal monochromators. A valid comparison is between the monochromated neutron current at resulution $\Delta\lambda$ at the sample position, and the time averaged neutron current at the sample position for the same wavelength resolution, over the useful wavelength range from λ_{min} to λ_{max} in the particular experiment.

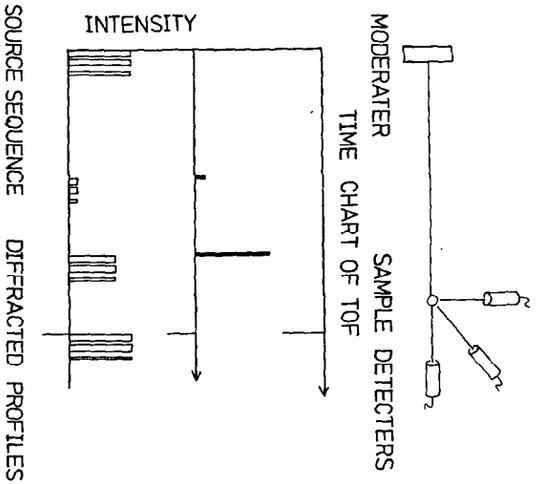


Figure A A diffraction (powder, single crystal or small angle) employing a pseudo-random sequence on the proton beam. Each diffraction pattern is identified from the sequence. The semi-pulsed nature of the source ensures that the "background of ignorance" from intense peaks does not contamnate weak peaks.

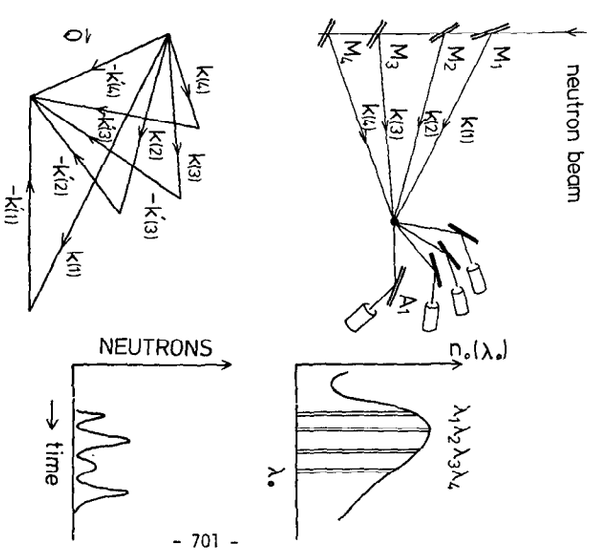
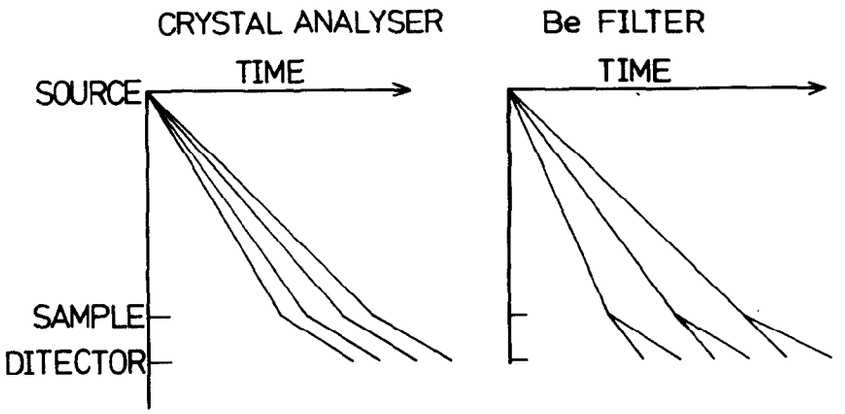


Figure B Coherent inelastic scattering on a long pulse source. The "three axis" spectrometer can use several different incomi wavelengths λ_1, λ_2, λ_3, λ_4. The excitations from each are roughly separated by time-of-flight.



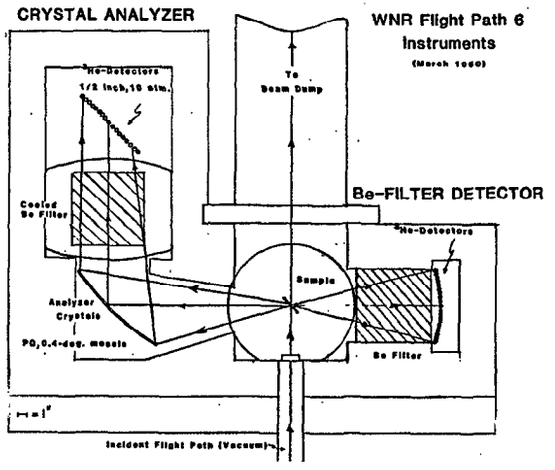


Figure D Two quite different types of incoherent inelastic spectrometers.

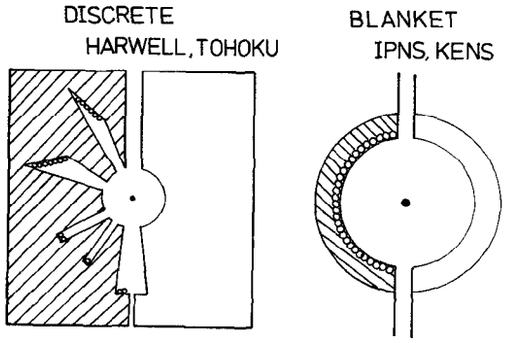


Figure C Two types of total scattering spectrometer.

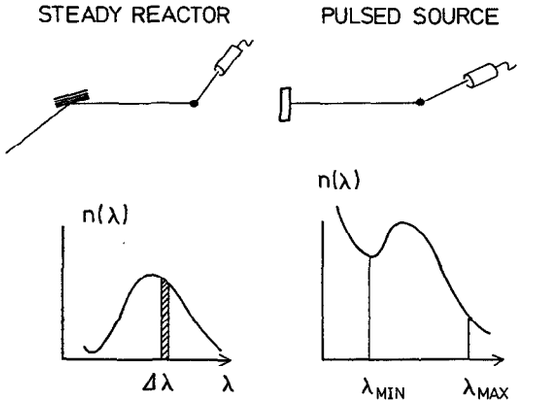


Figure E The comparison between reactor and pulsed source diffraction depends on the neutron current at the sample. The reactor monochromatic current can be compared with the time-averaged pulsed current at the same resolution $\Delta\lambda$ over the useful range of wavelengths.