ICANS-XIII
13th Meeting of the International Collaboration on
Advanced Neutron Sources
October 11-14, 1995
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

OPTIONS FOR NEUTRON SCATTERING INSTRUMENTS ON LONG PULSE NEUTRON SOURCES

Günter S. Bauer

Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

ABSTRACT

Instrumentation on long pulse sources can be approached either by instruments from short pulse sources and hence using mainly inverted time of flight techniques or by adopting reactor type instruments and making use of the time dependence of the source flux to enhance their performance substantially. While the first approach requires more or less single use of a beam line by one instrument, the second one allows multiple use of neutron guides, as customary on reactors and hence can make much better use of the source with gains up to 100 for time of flight spectrometers. To a certain extent, the design parameters of the source depend on which of the two approaches is chosen.

1. Introduction

While the scientific opportunities offered by neutron sources of different designs are - and should continue to be - the main line of arguments, cost effectiveness of their exploitation is another important issue. In this context long pulse neutron sources certainly have a certain leadway over short pulse sources, especially in the medium-to-high beam power regime (above a few Megawatts) [1], where a short pulse neutron source requires a linac capable to accelerate a sophisticatedly chopped beam of H^--ions and one or several rings to compress the linac macropulses into the desired short pulses. The design of the target and its surroundings is much more difficult for a short pulse source than for a source whose pulses are 200 µs long or more. The linac (no rings are required) for such a source can run on protons (suitable ion sources are available) and does not require chopping its macropulses, which is not only a significant technical simplification but also results in higher operating efficiency and probably in better reliability. Also, on the target side the mechanical load from long pulses is much smaller than from short pulses [2] which, if perhaps not a feasibility issue, will certainly affect the life time of the target and hence cost and availability of the source.

It is important, however, to keep in mind that short pulse neutron sources can offer certain possibilities in the use of epithermal neutrons and in very high resolution measurements which are unique and hence cannot be the subject of a debate on cost-effectiveness. Recent arguments on this subject therefore have concentrated more on the comparison in cold

Keywords: Instruments, time of flight, multiplexing, long pulse

neutron scattering and have been made on an instrument-to-instrument basis, using reactor instruments as the standard [3].

One problem of such a comparison is that, on the long pulse source, extensive use of inverse (or indirect) time of flight techniques has been assumed, whilst many of the reactor instruments are based on crystal monochromators. This not only leaves some ambiguity in the comparison (as manifest from the range in gain factors given for several of the instruments) but also does not account at all for the degree of source utilization, namely the number of instruments that can be accommodated at a source. The fact that the high flux reactor at ILL offers about 50 instrument locations whereas there are less than 20 on ISIS, has to do with the kind of technique used. It is the purpose of this paper to intensify the discussion on the options offered by adoption of essentially reactor-like instruments, which are well understood, to the opportunities of a time structure of the source. Clearly, most of these arguments are not really new. They have been extensively discussed in the context of the German SNQ-project a decade ago [4], [5], [6], but the present renaissance of the long pulse source enthusiasm seems to largely ignore them.

2. Energy selection in neutron scattering instruments

All neutron scattering instruments require some kind of energy selection in the beam incident on and/or scattered from the sample in order to obtain the desired information on momentum and energy transfer in the scattering process. The two traditional methods to accomplish this energy selection are Bragg-reflection from a crystal and selection by time of flight after a common starting time. Depending on which method is used, we can class the instruments according to Table 1, which also summarizes some of the consequences associated with the different selections.

Table 1: Beam utilization for different classes of neutron scattering experiments

Class of instrument	**Technique**	**Primary energy selection**	**Secondary energy selection**	**Comments**	
Crystal spectrometer (-diffractometer)	mono-chromatic incident beam	Crystal	Crystal none (diffr.)	Multiple use use of beam or guide	Sample in monochromated beam
Direct time of flight spectrometer		Crystal Choppers	TOF	End position	
Inverted time of flight spectrometer (-diffractometer)	"white" incident beam	TOF	Crystals none (diffr.)	Single use of beam or guide	Sample in direct beam

Since we can safely assume that, on a long pulse source, intensive use will be made of neutron guides, which can be quite effective also for thermal neutrons when coated with supermirrors, we will discuss very briefly the situation for this cases only.

The characteristic feature of a neutron guide is that the transverse momentum in both directions, Δk_x and Δk_y is constant for all neutron energies. This leads to a momentum distribution of constant width Δk_x and Δk_y and a variable length k_z, as shown in Fig. 1.

When momentum selection is done by time of flight with constant time intervals, the momentum interval selected, dk_z, is proportional to k^2. The intensity contained in each interval depends on the phase space density in the neutron guide, which is shown

(Maxwellian part of the spectrum only!) for two different moderator temperatures, namely 35 K and 350 K (note, that the curve for 350 K has been multiplied by a factor of 10!)

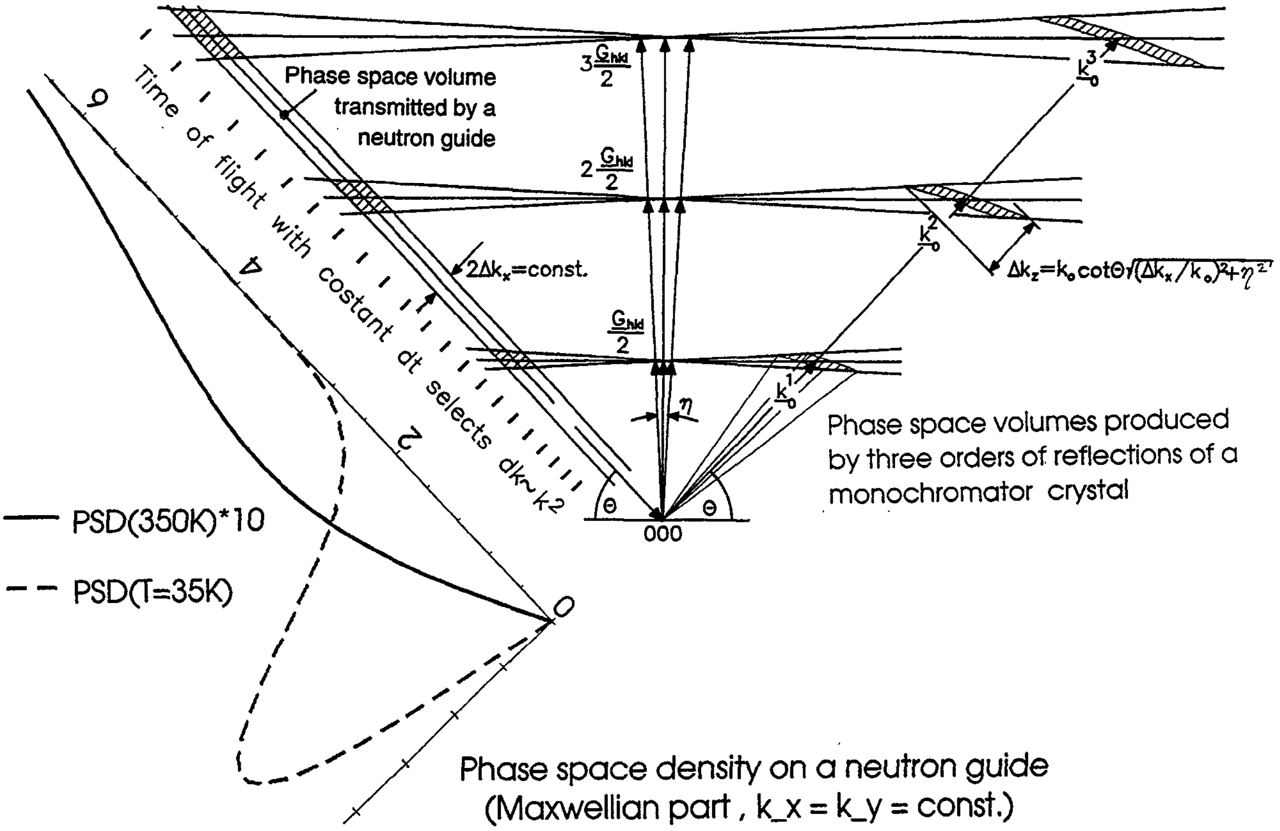


Figure 1: Neutron momentum selection at a neutron guide

Also shown is the situation for a monochromator crystal (or a multilayer, for small k_z), which deflects the beam by an angle of 2θ, with three orders. The angular mosaic spread causes the reflected beam to be fanned out in the transverse direction (vastly exaggerated in the figure for clearity) and also affects the width in Δk_z, which is otherwise proportional to k_0 and cot θ.

These differences must be borne in mind when comparing instruments using the two techniques but, as usual, the different characteristics can also be exploited beneficially in different ways.

For example, if Bragg reflection is used for energy selection, the time structure offers the opportunity to discriminate between the different orders of reflection and to either suppress their effects or use them in a convenient way. Collimators can be used to affect the instrument resolution in a flexible way. On the other hand, if energy selection by time of flight is used, the resolution can be affected by the pulse width and the distance L between the source and the detector.

At reasonable distances L of up to 40 m the pulse width offered by a long pulse source usually does not give good enough resolution. As a consequence a chopper system must be used to tailor the pulse. This poses several problems:

1. It is in general difficult to chop a wide beam (neutron guide) cross section with sufficiently short pulses and at high transmission. The solution to narrow the beam down at the chopper position by a tapered supermirror neutron guide and bring it back to more or less parallel rays by the opposite procedure may seem a way out at the first glance, but apart

form the technical difficulties, this requires that the neutron guide itself must have a significantly smaller angle of total reflection than the tapered sections, which counteracts their use for thermal neutrons where only supermirror guides will transmit a sufficiently large beam divergency.

2. As can be seen from Fig. 2, a chopper placed at a certain distance form the moderator (say at 4 m, which is well inside the target shield of a spallation neutron source) will have a pinhole effect, imposing an intensity modulation on the wavelength band transmitted, that reflects the pulse shape at the moderator.

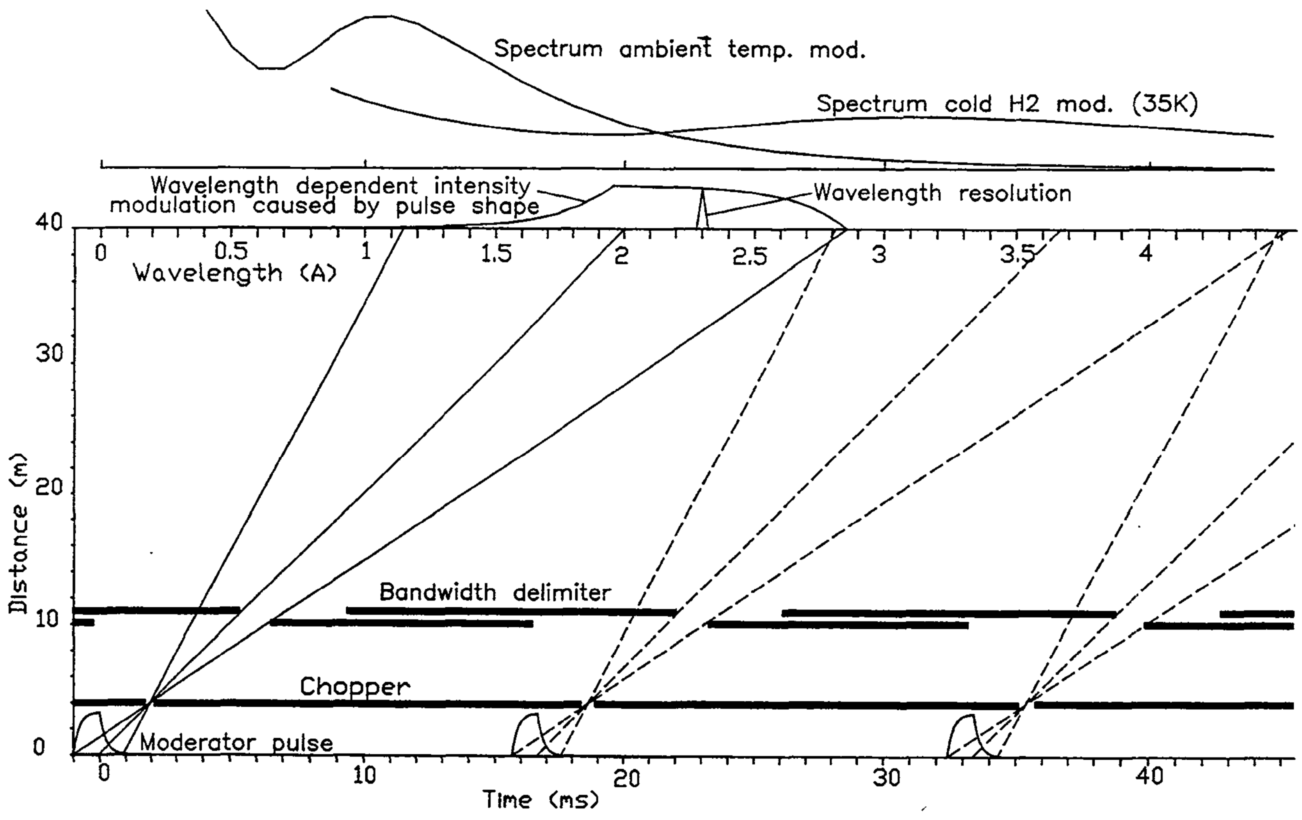


Figure 2: Space-time diagram for a pulsed neutron source with 1 ms pulse length and a chopper at 4 m from the moderator. In the example the chopper phase is shown set for 2.3 Å neutrons. The spectral distributions shown correspond to the first source pulse and do not account for wavelength-dependent transmission of the guide.

A band width delimiter (2nd chopper system) can be used to suppress those parts of the wavelength band which correspond to the trailing edge of the pulse (and to avoid frame overlap). The question whether the time between two pulses can actually be filled depends on the distance L chosen (as required by the desired resolution) and on the length of the proton pulse. Increasing the latter on the expense of the pulse current results in a lower peak-to-average intensity and hence has no benefit on the overall data taking rate. It simply increases the kinematic range of the scan which could otherwise be covered by selecting a different chopper phase (if needed; if not, this is a gain in measuring time!). On the other hand, increasing the pulse length and simultaneously reducing the repetion rate makes thermal cycling problems more severe and may well become a feasibiltiy issue at higher power levels (a few MW).

3. Even in those cases, where the full moderator pulse length gives sufficient resolution, such as small angle scattering [7], [8] and reflectometry [9], it is necessary to install more than

one chopper system in the guide to suppress frame overlap and penumbra effects, as can be seen from Fig. 3.

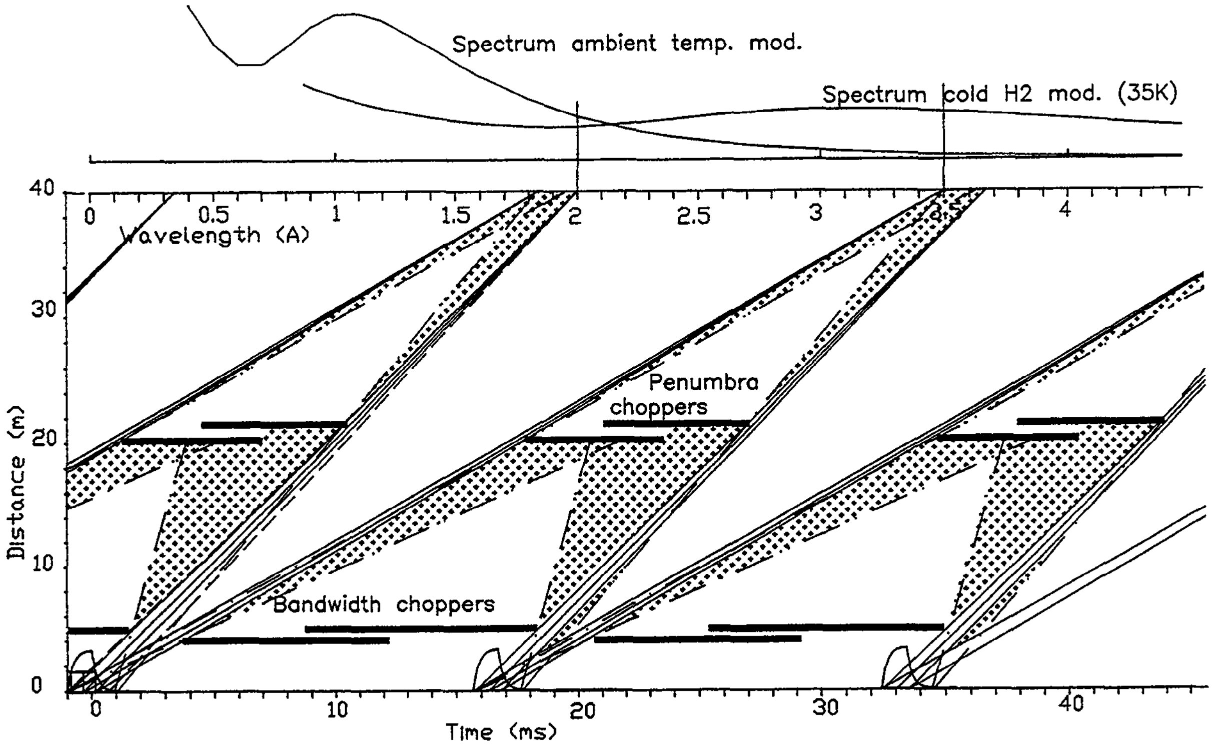


Figure 3: Space-time diagram for „long pulse“ experiments with about 5% resolution for neutrons between 2 and 3.5 Å at 40 m from the moderator. At least two chopper systems are required to suppress frame overlap and penumbra effects.

In summary, using long source pulses to perform a time dependent energy selection on the incident beam requires a large technical effort, is limited in its usefulness and makes each guide unique for the instrument it is designed for. It also requires to locate the samples in the direct beam which further impedes multiple use of a guide and thus places a high share of the total facility cost on each instrument. The gains in measuring time often quoted for indirect ToF methods frequently result form the use of a large solid angle at the analyser side which, in addition to the proprietary use of a guide and the chopper system, adds significantly to the cost of such instruments. The question, whether this also produces useful information certainly depends very much on the problem under investigation (see below).

Another option is to use direct time of flight also on a long pulse source, similar to how it is done on a reactor, i.e. with a monochromator crystal and a chopper in the „monochromatic“ beam and a detector system covering a large solid angle.

The first and most obvious advantage of this method is that the monochromator is placed in the intense beam of the neutron guide, rather than the sample. This makes multiple use of the guide easy. It may also have an effect on sample-generated backgrounds: If the sample is in the „white“ beam much more parasitic scattering will occur in the sample than if it is hit only by the much smaller intensity of the monochromatic beam. For highly radiation sensitive samples this may even be an important issue relating to the effects under investigation ("in vivo") experiments.

In direct ToF-experiments the gain over a cw-source is easy to quantify. In the first approximation it is given by the peak-to-average flux ratio, multiplied by the source utilization ratio, i.e. the ratio of actual pulse repetition rate to the optimum one chosen on a pulsed source. It will be higher, if the source pulses are shorter and the repetition rate of the source is higher. This issue was discussed extensively in a previous paper [1].

It may not always be possible to come sufficiently close to the optimum repetition rate with a long pulse source. There exists, however, the option to use more than one incident wavelengths, if the frames are long. This is shown for the case of a monochromator crystal in Fig. 4. A chopper has been introduced, which, rather than suppressing the second order of the monochromator reflection, allows it to pass on to the sample - well separated in time due to the distance from the moderator chosen. In this case, two different kinematic regions are covered simultaneously in one experiment (cf. Fig. 6).

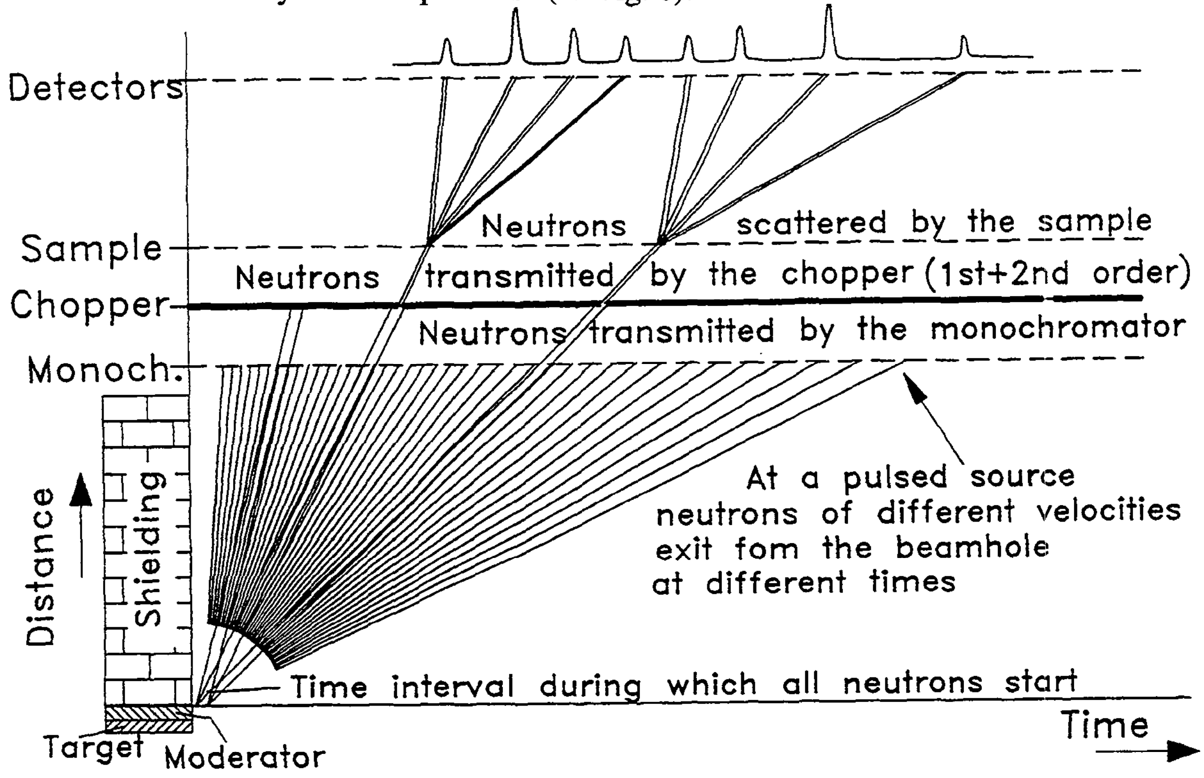


Figure 4: Space-time diagram for a direct ToF-spectrometer on a long pulse source using two orders of the monochromator reflection.

It is, of course, not necessary to use a monochromator in order to exploit more than one incident energy on a direct ToF-spectrometer. If an end position on a guide is available, a chopper system can in principle be used to select the incident energies. In this case no „higher order“ restriction applies to the second energy chosen. It will simply be determined by the opening times of the chopper system.

At constant time average flux (same beam power and moderator-reflector configuration) the peak flux $\hat{\phi}$ is

$$\hat{\phi} = \bar{\phi} \cdot \frac{1}{f \cdot t_p}\left(1 - \exp\{-t_p / \tau(\mathrm{v})\}\right) \qquad (1)$$

where t_p is the proton pulse duration and $\tau(v)$ is the life-time of neutrons of velocity v in the moderator. f is the source repetition rate and $f \cdot t_p$ is the duty cycle, which is assumed to be constant. If a chopper system rather than a monochromator is used to select more than one wavelength this requires, as a consequence of the pinhole effect shown in Fig. 2, a long t_p in order to have sufficient intensity at all incident wavelengths and hence results in a much smaller $f\cdot\hat{\phi}$. Furthermore, fast choppers which control a large beam cross section near the moderator are a formidable task!

Clearly, for very low incident energies the choice of monochromators is restricted and the question whether to use direct or indirect time of flight involves more than only the issue of multiple use of guides and time utilization. While we are not going to deal in detail with questions of resolution, it seems appropriate to look at the kinematic range covered in the two techniques.

3. Scattering kinematics in direct and indirect time of flight techniques

It is customary to show the kinematic range covered by a scattering experiment as a function of Q and $\hbar\omega$. This is a helpful representation to give a quick overview, in particular if dealing with isotropic or polycrystalline samples, where no dependence of the scattering law on the direction of $\underline{Q}$ can be measured.

In fact, the conditions of conservation of energy

$$\Delta E = \hbar\omega = \frac{\hbar^2 k_i^2}{2m} - \frac{\hbar^2 k_f^2}{2m} \tag{2}$$

and of momentum

$$\underline{Q} = \underline{k}_i - \underline{k}_f \tag{3}$$

define a set of parabolae in the $\underline{Q}$-ω-space (on the surface of a paraboloid), whose apex is given by the energy of the incident neutron $\left((\hbar\omega)_{\max} = E_i = \frac{\hbar^2 k_i^2}{2m}\right)$ and whose orientations in the Q_x-Q_y-plane are determined by the scattering angle ϕ_s at the sample (Fig. 5).

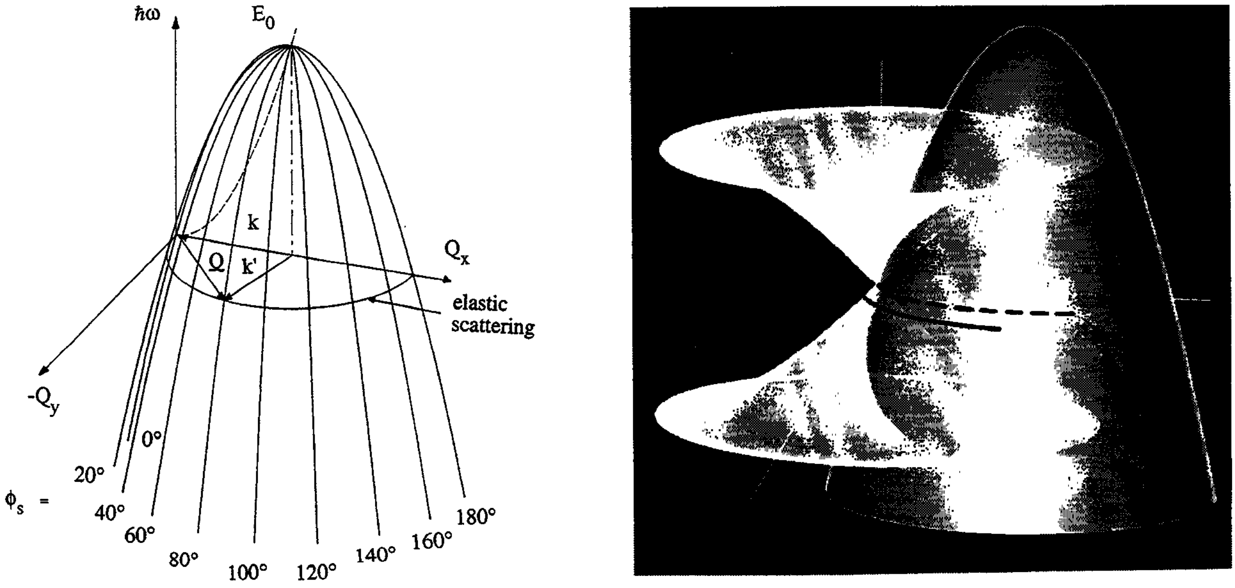


Figure 5: The kinematic range of a scattering experiment in the $\underline{Q}$-ω-space. Scattered intensity can be measured, when the scattering law intersects with the kinematic surface, as shown schematically in (b).

In a direct time of flight experiment the scan is along those parabolae which correspond to the individual detector settings at different scattering angles ϕ_s. The variation of Q as a function of time is along a line in the Q_x-Q_y-plane starting at the end point of the $\underline{k}_i$-vector and including an angle ϕ_s with this vector (bottom part of Fig. 6a). The Q-range covered is determined by the area between two circles centered around the end of k_i and having radii equal to the highest and lowest neutron momenta that can be analysed with sufficient resolution. For each point in Q a unique value of $\hbar\omega$ can be measured, depending on k_i. The Q-$\hbar\omega$ representation mentioned above is obtained by a rotation of all Q-vectors around the origin of the reciprocal space into the plane defined by $\underline{k}_i$ and $\hbar\omega$ (top part of Fig. 6). The curves are then described by:

$$Q^2 = \frac{2m}{\hbar^2}\left(2E_i - \hbar\omega - 2\cos\phi_s\sqrt{E_i(E_i - \hbar\omega)}\right) \tag{4}$$

Fig. 6a shows these curves for k_i = 2 Å^{-1} and 4 Å^{-1}, corresponding to two orders of reflection from the same monochromator crystal.

Although these facts are of course well known, it is important to keep them in mind when discussing the comparison between direct and indirect ToF techniques.

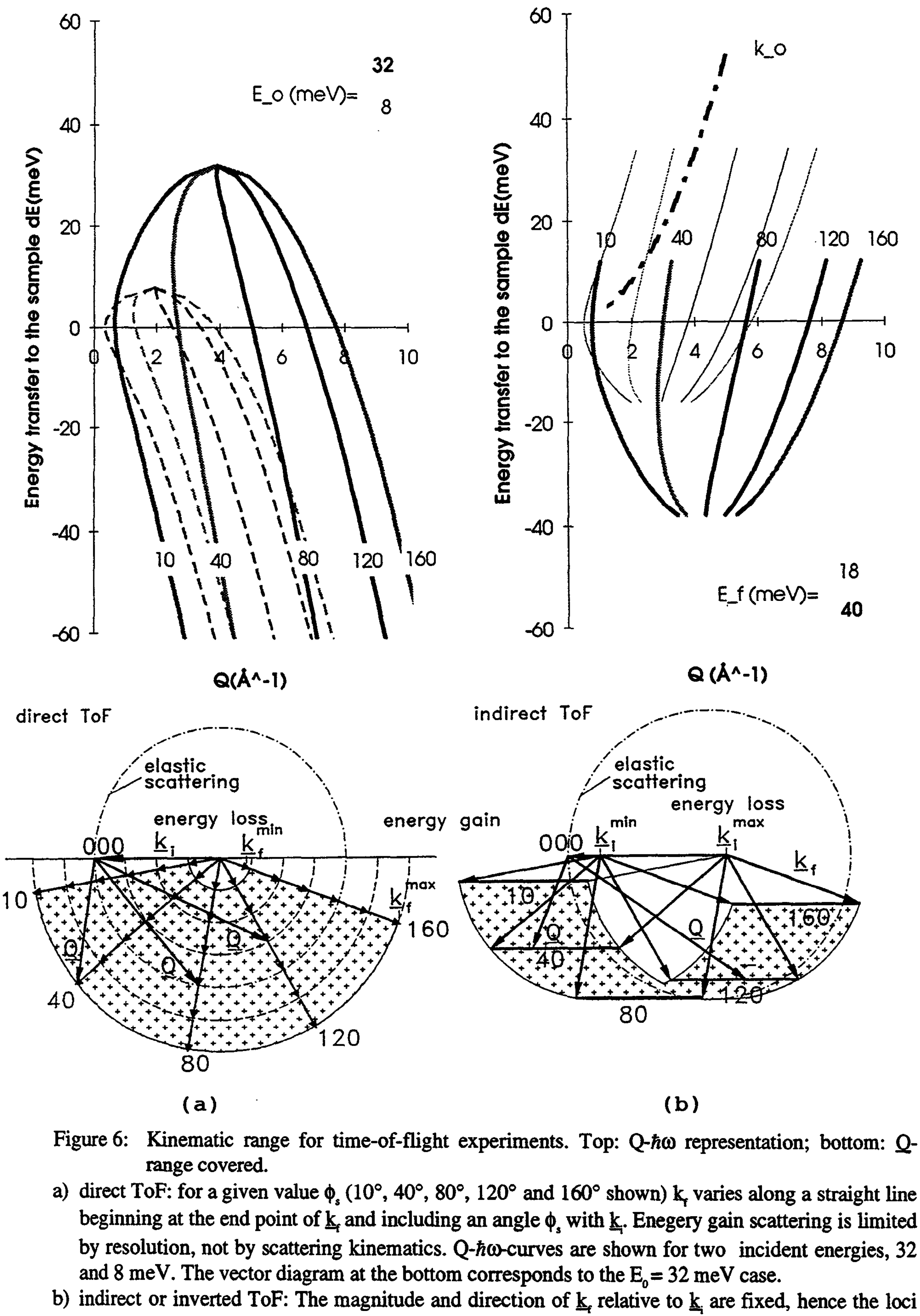
In an indirect ToF-experiment with crystal analysers set at a fixed value k_f the incident energy and hence the position of the kinematic scattering surface varies with time, the apex moving on a curve given by $(\hbar\omega)_{\max} = E_0 = \frac{\hbar^2 k_i^2}{2m}$, the dispersion relation of the incident neutrons.

The loci for measurable combinations of energy- and momentum transfer are then obtained by introducing $E_f = E_i - \hbar\omega$ into eqn. (3) and are shown in Fig. 6b for the case of k_f = 3 and 4.5 Å^{-1}, and 1 Å^{-1} < k_i < 5 Å^{-1} (a reasonable range for a room temperature moderator according to Fig. 1).

Also shown in the bottom part of Fig. 6b are the scattering triangles for different times (values of k_i) corresponding to different scattering angles ϕ_s (10, 40, 80, 120 and 160°). It is obvious that the Q-vectors corresponding to a given scattering angle now lie on a line parallel to $\underline{k}_i$. If the k_f-values are the same for all ϕ_s, there is still a unique correspondence between Q and $\hbar_\omega$ that can be measured. From Figs. 6a and 6b it is clear that the coverage of the Q-space is different in the two techniques.

It is also obvious that, for indirect ToF-experiments the $\hbar\omega$-range is limited on the energy loss side of the neutron (positive values of $\hbar\omega$) by the maximum useful k_i and on the energy gain side by k_f. In direct ToF, the energy loss side is limited by k_i (and the time one is prepared to wait for down-scattered neutrons to arrive at the detector), while the limit on the energy gain side will be set by the resolution of the experiment.

Certain advantages for inverted time-of-flight techniques arise from the fact that the detectors will not see neutrons that have lost almost all of their energy and hence take a long time to arrive, eventually leading to frame overlap problems in direct ToF. They also cover a large Q-range for energy loss scattering of the neutron and hence depend less on the state under investigation to be occupied in the sample. On the other hand, while in direct ToF-experiments a k_i-value can be chosen that represents a high phase space density and the full peak height of the source pulse, the intensity associated with the different k_i in indirect ToF



(a) (b)

Figure 6: Kinematic range for time-of-flight experiments. Top: Q-$\hbar\omega$ representation; bottom: $\underline{Q}$-range covered.

a) direct ToF: for a given value ϕ_s (10°, 40°, 80°, 120° and 160° shown) k_f varies along a straight line beginning at the end point of $\underline{k}_f$ and including an angle ϕ_s with $\underline{k}_i$. Enegery gain scattering is limited by resolution, not by scattering kinematics. Q-$\hbar\omega$-curves are shown for two incident energies, 32 and 8 meV. The vector diagram at the bottom corresponds to the $E_0 = 32$ meV case.

b) indirect or inverted ToF: The magnitude and direction of $\underline{k}_f$ relative to $\underline{k}_i$ are fixed, hence the loci for $\underline{Q}$ lie on lines parallel to $\underline{k}_i$, as k_i varies. Examples shown pertain to ϕ_s = 10, 40, 80, 120 and 160°. Energy gain scattering is limited by the intensity distribution in the incident beam.

For both cases the $\underline{Q}$-range is shown by the shaded areas in the bottom part of the Figure. The condition for elastic scattering ($k_f = k_i$) gives the dash-dotted circles. $\underline{Q}$-values inside these circles are possible for energy loss of the neutrons, outside the circles for energy gain.

values not only represents the variation of the phase space density in the moderator, but also is subject to the pinhole effect by the chopper as shown in fig. 4, unless the source pulse is very long.

It is well known that by a suitable choice of k_f as a function of the scattering angle ϕ_s the loci for the $\underline{Q}$-vectors coverd for different ϕ_s can be shifted to the same distance from k_i („PRISMA“-condition: $\sin(\phi_s)_n/\sin(\vartheta_A)_n = \text{const}$, with $(\vartheta_A)_n$ being the Bragg-angle for the n-th analyser). This option has been extensively discussed recently [12], [13] and can, in certain cases, be used to produce energy transfer scans for a fixed value of $\underline{Q}$ (or $\underline{q}$), i.e. to simulate constant $\underline{q}$-scans on a triple axis spectrometer. In practice, however, several difficulties may arise:

If one tries to set the spectrometer up such that the scanning line in $\underline{Q}$ coincides with a high symmetry direction in the crystal lattice, the choices are very restricted, because (a) every particular distance from the k_i-vector requires a unique set of analyser energies (k_f-values), (b) small k_f's are not easily accessible in practice due to the large Bragg-angles required, which cannot be realized in a multi-arm arrangement with closely spaced analysers, (c) large k_f's lead to poor resolution because of the small deflection angles at the analysers, and (d) the spacing between the $\hbar\omega$-values measured is determined by the angular spacing of the analyser arms and cannot easily be matched to the width of the peaks to be measured.

In summary, while it is clear that inverted ToF inelastic scattering has certain merits, the question, whether such an instrument should occupy a beam line of its own on a long pulse source must be considered very carefully because the alternative of a direct ToF-machine or triple axis spectrometer using a shared beamline may often offer even better opportunities.

4. Polarization effects - ToF versus TAS

One problem which makes time of flight techniques difficult to use in single crystal investigations is the question of the polarization of the elementary excitations or magnetic scattering relative to $\underline{Q}$. It is obvious from the dynamic structure factor

$$F_{dyn}^2 = \sum_{l=0}^{n} \left(b_l / \sqrt{M_l} \cdot \underline{Q} \cdot \underline{e}_l(q,i) \exp\left(i\underline{Q} \cdot \underline{\rho}_l \right) \exp\left(-W_l \right) \right) \tag{5}$$

and the magnetic scattering cross section

$$\left(\frac{d\sigma}{d\Omega} \right)_{mag} = \left(\frac{p}{\mu_p} \right) \left| < \underline{Q} x \left(\underline{\hat{M}} x \underline{Q} \right) > \right|^2 \tag{6}$$

that, in order to obtain clear quantitative results, $\underline{Q}$ should be oriented parallel to $\underline{e}_l$ in inelastic nuclear scattering and perpendicular to the Fourier transform of the magnetisation vector, $\underline{\hat{M}}$, in magnetic scattering. In ToF-measuremtns the direction of $\underline{Q}$ varies in a scan for each detector and the above condition can only be fulfilled for a range of $\underline{Q}$ by regrouping data from different detectors measured at different times. While this may be possible in direct ToF, with the detectors spaced closely enough, few directions exist in indirect ToF, where this is possible, as can be seen from the bottom part of Fig. 6a and b.

The best instrument to fulfill his condition is a triple axis spectrometer (TAS) which, as soon as the large kinematic range covered in time of flight cannot be fully exploited, becomes highly competitive. A TAS, too, uses a crystal monochromator and hence can share a neutron guide with other instruments. On a long pulse source, the time structure can be exploited to enhance its performance significantly relative to a continuous source by suppression of spurious effects and background through a time gate at the detector [1].

This option poses no particular restrictions to the time structure of the source, but it will be the more effective, the shorter the pulses and the higher the intensity per pulse. It is, however perfectly compatible with a 100 Hz repetition rate and a pulse width of 200 µs, which would be a desirable set of parameters also for direct ToF-instruments. (A high pulse repetition rate also reduces thermal cycling loads on the system components of the source, which, as noted before, is a decisive advantage).

There will be many instances where the much higher gain factor that can be obtained for direct time of flight methods on such a source (of the order of 40) compared to triple axis machines (of the order of three), make it easier to perform certain research tasks by ToF rather than by TAS. This will certainly lead to a different "population structure" on a long pulse source than on a continuous source, but the principal character of the inelastic scattering instruments can remain the same.

5. Correlation ToF-Techniques

High intensity (long) pulsed neutron sources have been recognized early on [14] to offer unique options for correlation techniques in time of flight. In addition to correlating a measured event to the chopper sequence(s), the on-off condition of the beam at the moderator can be used to screen against the high background which otherwise plagues the technique on a cw-source. In the mean time the concept of inverse Fourier time of flight instruments has been developed to a high degree of perfection [10], [11].

For inelastic scattering the crucial advantage is that there is no need to fix k_f by crystal analysers. With two Fourier choppers of different grating and running independent of each other, the k_i and k_f values that shall be related to one another can be chosen virtually at random and independent of each other. This does not only allow to simulate the "PRISMA"-condition ($k_f \cdot \sin \phi_s = \text{const}$) on a long pulse source with a resolution indepent of the pulse length and with every desired line in reciprocal space easily achievable, it also makes the very interesting mode possible, where k_i/k_f is constant for every detector. This results in a scan where the locus for $\underline{Q}$ is a straight line through the origin of the reciprocal space. Adjusting k_f for the different detectors properly will make all these lines coincide and enable a complete longitudinal phonon scan along a high symmetry direction to be performed in a single run. By the same token, the condition $\underline{Q} \perp \underline{\hat{M}}$ (eqn. 6) can be fulfilled for the whole set of detectors and incident scattering vectors.

With regard to transversely polarized phonons, a constant q scan should also be possible, but only one pair of k_i-k_f values will contribute for each scattering angle ϕ_s.

The criterion that needs to be fulfilled is

$$Q^2 = k_{i,n}^2 + k_{f,n}^2 - 2k_{i,n}k_{f,n}\cos\phi_{s,n} \tag{7}$$

with n designating the detecor number. This will require the use of variable time channels and predelay times but should be feasible with a predetermined measuring program for each value of $\underline{Q}$. If the opportunity exists to carry out more than one correlation program for each detector, several constant Q-values can be selected simultaneously.

The opportunities offered by this method have so far not been fully exploited in practice because of the lack of suitable sources; on cw-sources the need to introduce a "long pulse" chopper costs too much intensity and on short pulse sources the average intensity has been low to begin with. It should be noted that the introduction of two Fourier choppers means that only about 1/16th of the pulse intensity (average flux) is actually used, albeit at very good resolution. While this is about what one would expect for a standard direct ToF-instrument on a long pulse source, it is less than what inverted ToF uses on a pulsed source.

With respect to constant $\underset{\sim}{q}$-scans, the technique uses 1/16th of the full average flux at each detector and $\underset{\sim}{q}$-value selected. In a very crude approximation it would then become competitive to a TAS, if more than 16/m detectors can contribute to the scan with m being the number of meaningful q-values examined simultaneously.

It is probably worth emphazising that a Fourier chopper is the only device which can generate very short pulses on a large beam cross section.

The power of this technique certainly justifies an end position on a guide or even single use of a beam hole.

6. Diffraction

For single crystal diffractometers more or less the same is true, as for triple axis spectrometers:

Using the (position sensitive) detector(s) in a time resolving mode will not only make filters unnecessary and reduce the background contribution, it will also allow to distinguish higher order reflections and thus improve the information content of the measurement. Again, a monochromator (or a set of monochromators, see below) is used and multiple utilization of a (supermirror) guide is possible.

In the case of powder diffraction it is beyond doubt that short pulse spallation sources have a decisive advantage because (a) in the slowing down regime the pulse width is inversely proportional to the neutron velocity and hence $\Delta v/v = \Delta d/d$ is constant and very good. Similarly high quality data can also be obtained in the Maxwellian part of the neutron spectrum if the moderator pulse is kept suitably short by poisoning and decoupling the moderator. The large scanning range in inverted time of flight diffraction easily compensates for the factor of roughly 20 in the pulse integral lost in comparison to an optimized coupled moderator, as would be used on a long pulse source.

On a long pulse source it is, however, possible to improve the situation for diffraction by taking advantage of the time structure and using not only several orders of one monochromator crystal but stacking two or more crystals to deflect more wavelength packets [1]. The corresponding distance-time diagram is shown in Fig. 7. Here, a C-002 and Si-220 monochromator were assumed, set at an angle of $2\ \theta_m = 130°$. As can be seen, good separation of the reflected wavelengths is obtained at a distance of 25 m even for 1 ms long proton pulses. A background rotor placed at the edge of the target shielding will reduce the overall background from fast neutrons while the pulse is on and will, at the same time, suppress the C-002-reflex, which would otherwise interfere with the Si-220 reflex of the following pulse. Clearly, if the (position sensitive) detector of the spectrometer is operated in a time resolving mode, the contributions from the different wavelengths can be easily distinguished and used to improve the measurement. Without any attempt to optimize the resolution or intensity, the resolution curves obtained for this situation were calculated [15] with the following assumptions given on the figure, where α_1, α_2, α_3, and β are the collimation angles in front of the monochromator, the sample and the detector respectively and β is the mosaic spread of the monochromator.

The result is shown in Fig. 8. It is obvious that in the d-range between 0.5 and 8 Å measurements with a resolution better than 2% can be performed. Between 0.4 and 2.5 Å a resolution better than 0.4 % is achieved. At the same time, most of the d-values are measured several times with different resolution, which should be valuable in sorting out wavelength dependent effects and carrying out a quantitative analysis of the intensities.

Again, while a standard powder diffractometer on a long pulse source will not be used to routinely solve complicated structures if a short pulse source (or an X-ray diffractometer) is available, there are many problems which do not require the large range in d-values. Those problems can be treated on the diffractometer described here with orders of magnitude better intensity.

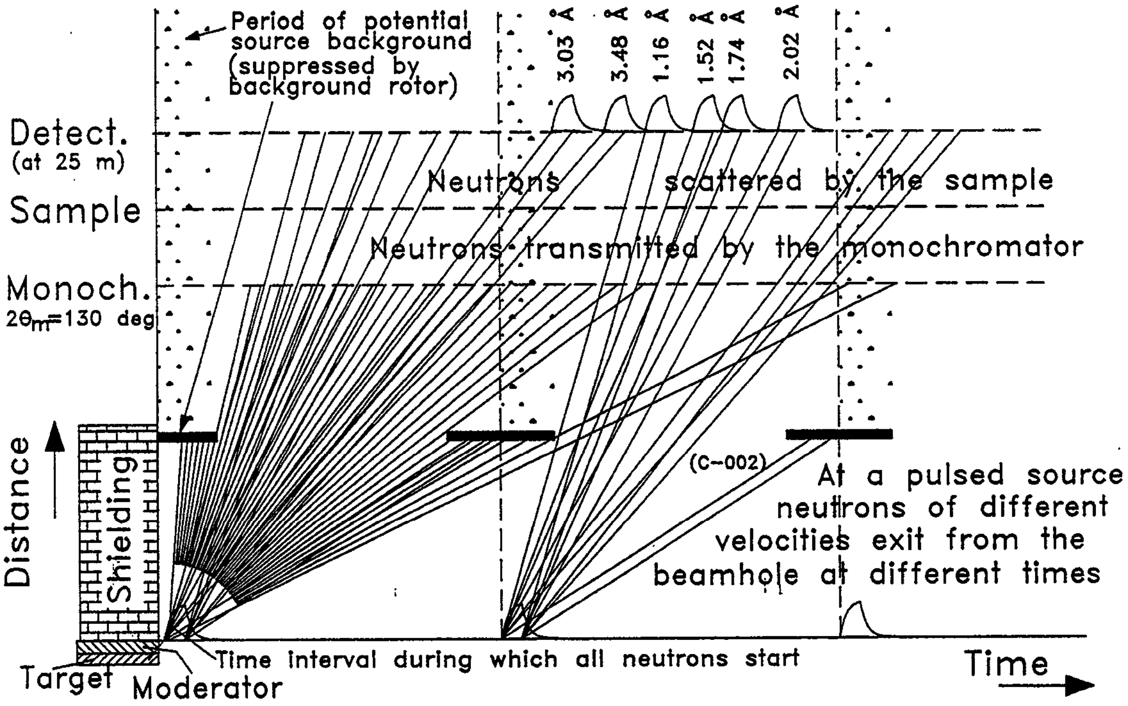


Figure 7: Distance-time diagram for a powder diffractometer with multiple monochromator on a pulsed source.

Although a collimator was assumed to be used in front of the monochromator, also this instrument can share a neutron guide.

Finally, it should be noted that the Fourier correlation technique mentioned in chapter 5 is, of course, also suitable for diffraction measurement. If used as total scattering instrument (as customary in diffraction), only one Fourier chopper is required and data taking is relatively straight forward, allowing very high resolution. The inelastic spectrometer with two Fourier choppers as outlined in chapter 5, however, allows to chose the condition $k_i = k_f$ for all detectors (with each scan running along a different line in Q-space) and to measure truely elastic or qusielastic scattering in a whole sector in reciprocal space simultaneously, using 1/16th of the time average flux of the source. Again, this instrument must occupy an end position of a guide or beam.

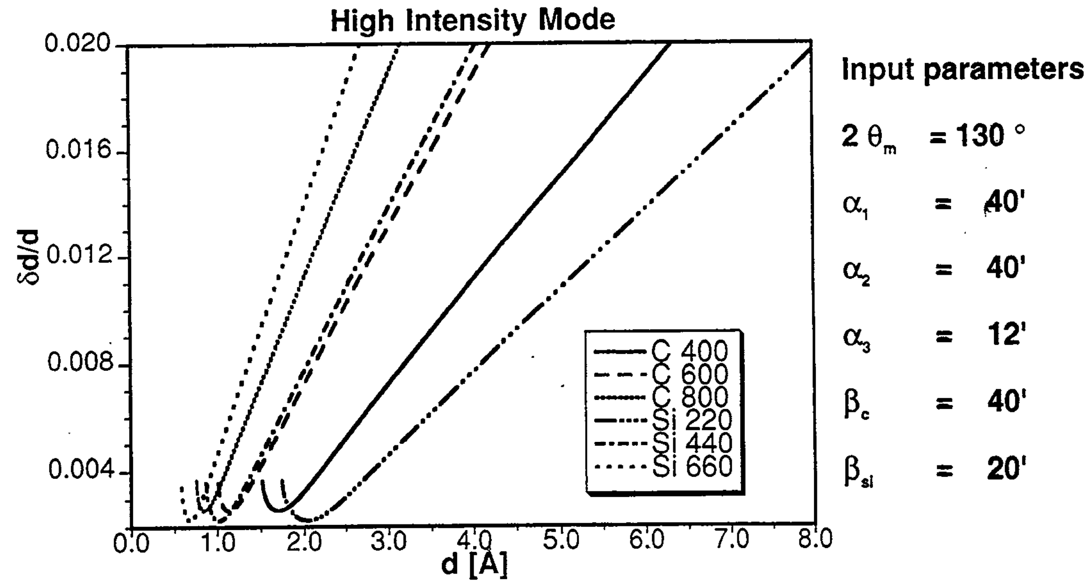


Figure 8: Multi-monochromator resolution functions in a high intensity mode of a powder diffractometer on a pulsed source.

7. Further options for multiplexing

The term "multiplexing" has been used to describe multiple use of the same pulse other than in inverted time of flight. Apart from the case of the powder diffractometer described above, also the simultaneous use of more than one pulses per frame in a direct ToF-spectrometer or a single crystal diffractometer would fall in this category. Other, more elaborate methods for multiplexing techniques have been proposed, such as the multicrystal-monochromator back scattering spectrometer "Musical" [5] where separation of closely neighbouring wavelengths is achieved by a "detour" through a stack of crystals in back scattering with appropriate mutual separation.

Other methods, using more high tech approaches have been developed by the group in Vienna hand have been described e.g. by Rauch [16]. We will not treat them in detail here. An overview over other options can be found also in [6]. The common features of these methods are that

- they provide useful neutrons practically throughout the frame between two pulses
- they are not very sensitive to pulse length but are most effectively applied for pulses of the order of 200 μs
- they can utilize the full intensity of coupled moderators with grooved surfaces
- they are applicable also at relatively high repetition rates, e.g. 100 Hz, which is favoured for direct ToF-techniques and from the point of view of thermal cycling.

8. Conclusions

Inverted time of flight techniques are the natural choice for short pulse spallation neutron sources, where they offer unique possibilities in powder diffraction, epithermal neutron spectroscopy and very high resolution spectroscopy on nearly dispersion-free modes. Trying to use the same techniques on long pulse sources either requires excessively long flight paths and low pulse repetition rates or difficult chopper systems and long pulses. One of the most important features of short pulse sources, the constant resolution due to the 1/v-dependence of the pulse width cannot be simulated in this way. They also imply more or less single use of a beamport by one instrument only and hence are not very cost effective. Their use should therefore be restricted to cases where no other alternatives exist. Long pulse spallation neutron sources can today be conceived with time average fluxes approaching those of the best existing high flux reactors and the most cost-effective way of using such sources is by multiple use of guides, as it has become standard practice on reactors. Also performance-enhancing techniques now in use of reactor sources, such as curved monochromators can be retained.

Practically all instrument types now in use at reactors can benefit from the time structure of a long pulse source by making more efficient use of the neutron beams and reducing backgrounds. While the gains will average around an order of magnitude if straight-forward improvements to the instruments are made, they will vary from one type of instrument to another approaching 100 for time of flight spectrometers. This will eventually lead to a different population of instrument types on a long pulse source compared to what we find at present reactors, driven by the best options to meet future scientific needs. As usual, new opportunities will trigger new developments. Some of them can already be seen on the horizon.

One important example are Fourier correlations techniques for which the pulsed nature of the source allows to overcome the background problems they suffer from on continuous sources, but which have no stringent requirements to pulse length. The important issue is that the decision on the future instrumentation affects the choice of parameters for the long pulse source: while inverted time of flight techniques prefer long pulses and low repetition rates, reactor-like methods can profit from shorter pulses and higher repetition rates. At the same time average beam power the second case makes the design of the linac and in particular of the target significantly easier because it reduces thermal cycling problems. If the source is fed from a ring accelerator which produces inherently short pulses, this will constitute a more difficult situation for the target, but will not affect the performance of the instruments adversely. On the contrary, for direct ToF-instruments the situation will be further improved and even neutrons in the slowing-down regime would become useable (albeit by inverted ToF-techniques!).

9. References

[1] G.S. Bauer "Some general reflexions on long pulse neutron sources" in *Proc. Int. Workshop on Long Pulse Spallation Sources Lawrence Berkeley Laboratory*, 18-21 April 1995 to be published. Submitted to J.N.R.(1995)

[2] K. Skala and G.S. Bauer "On the Pressure Wave Problem in Liquid Metal Targets" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proceedings 95-02 (1995)

[3] R. Pynn and L. Daemen "The Performance of Neutron Spectrometers at a Long-Pulse Spallation Source" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proceedings 95-02 (1995)

[4] G.S. Bauer, "The general concept for a spallation neutron source in the Federal Republic of Germany"; *Atomkernenergie-Kerntechnik* 41 (1982) p.234-242

[5] R. Scherm, B. Alefeld "Instruments for High Flux Sources with Time Structure of Neutron Flux" paper *IAEA-CN-46/80* in "Neutron Scattering in the 'Nineties", *IAEA conference procceedings, Vienna*, (1985) p. 247-259

[6] G. S. Bauer, R. Scherm, "Forthcoming Instrument Developments for Improved Utilization of Neutron Beams"; in "Neutron Scattering", *Proc. Int. Conf. Santa Fe*, physica 136B (1986), p 80-86 North Holland, Amsterdam

[7] H. Conrad "On Proton Pulse Lengths and Rep. Rates with Emphasis on SANS" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proceedings 95-02 (1995)

[8] Glenn A. Olah, Rex P. Hjelm and Phil A. Seeger "Small-Angle Scattering Instruments on a 1 MW Long Pulse Spallation Source" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proceedings 95-02 (1995)

[9] M.R. Fitzsimmons and Roger Pynn "The Performance of Reflectometers at Continuous Wave and Pulsed Neutron Sources" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proc. 95-02 (1995)

[10] P. Hiismäki "Principles of Reverse Time-of Flight Method an Fourier Technique" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proceedings 95-02 (1995)

[11] V.L. Aksenov, A.M. Balagurov, V.A. Trounov and P. Hiismäki "Performance of the High Resolution Fourier Diffractometer at the IBR-2 Pulsed Reactor; Latest Results" *Proc. ICANS-XIII, Paul Scherrer Insitut*, PSI-Proc. 95-02 (1995)

[12] B. Dorner "A Comparison of Time-of-Flight (TOF) and Three Axis Spectrometer (TAS) Techniques for the Study of Excitations in Single Crystals" *Journal of Neutron Research* 2 (1994) 115-127

[13] M. Hagen, U. Steigenberger, C. Petrillo and F. Sacchetti "Future opportunities and present possibilities for coherent inelastic single crystal measurements on pulsed neutron sources" to be published in *Nucl. Inst. Meth.*

[14] G.S. Bauer, H. Sebening, J.-E. Vetter, and H. Willax (eds.) "Realisierungsstudie zur Spallations-Neutronenquelle" report Jül-Spez-113 and KfK 3175 *Kernforschungsanlage Jülich und Kernforschungszentrum Karlsruhe* (1981), p. 129

[15] P. Fischer, private communication

[16] H. Rauch: 'Novel beam bunching methods by perfect crystals and electromagnetic means' paper IAEA-CN-46/40 in *"Neutron Scattering in the 'Nineties"*, *IAEA conference procceedings*, Vienna, (1985) p. 35-52