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BACKSCATTERING SPECTROSCOPY WITH 2 μeV RESOLUTION AT PULSED SPALLATION SOURCES

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The energy resolution of standard, established IRIS type inverted geometry time-of-flight backscattering (TOF-BS) spectrometers at pulsed spallation sources amounts to about 15 μeV using graphite analyzer at 6.7 Å wavelength in contrast to typical continuos source instruments, which provide 1-2 μeV resolution Si(111) crystal analyzer at 6.27 Å. By the IRIS type technique this kind of high resolution can only be achieved by mica analyzers at about 19 Å wavelength at the expense of a large losses in beam intensity and available momentum transfer range. It is shown in this work that by adding an optional fast chopper at some 5 m from the moderator and using Si analyzer crystals on an IRIS type instrument, a resolution close to that of the continuous sources machines can be attained at very competitive intensities and without the above drawbacks of going to 19 Å wavelength. The performance of an apparatus with the basic dimensions of IRIS and operating on a partially coupled cold moderator with 150 μs FWHM pulse length at the upgraded LANSCE source was quantitatively evaluated using detailed Monte Carlo simulation.

1. Introduction

In high resolution neutron spectroscopy one crucial requirement is to be able to tune the resolution. This implies, that depending on the behavior of the sample studied one has to have the freedom of trading resolution for intensity and vice versa. This flexibility is one of the keys of the historic success of triple axis spectroscopy (TAS). Continuous source (CW) TOF spectrometers are also easily tunable in resolution by changing the chopper speed or, more recently, by choosing the width of the chopper window. With the pulse width determined by the source moderator, spallation source instruments of the by now established design lack this flexibility, which is a substantial drawback. The resolution of backscattering spectrometers, CW or pulsed, is not easy to tune anyway, since it requires changing the whole set of analyzer crystals. It is nevertheless a standard approach to share the covered solid angle between two sets of different analyzers of different resolutions. Both from economical point of view and from that of reliable data collection it is preferable to have the flexibility of adapting the resolution to the requirement of the experiment on the same instrument, as opposed to operating several similar instruments with different resolutions. On pulsed sources the latter, less favorable solution appears most often to be the only option, in view of the handicap of not being able to change the pulse length and intensity of the moderator chosen once for ever (or at least for many years).

This sizable drawback of pulsed spallation sources can be overcome by a simple, but by now never implemented technique of using an optional chopper upstream in the beam in order to shorten, if needed, the pulse length of the moderator chosen to be optimized for highest intensity. Without this (and a number of other innovative techniques, a good number of them already proposed, but not yet tested) pulsed spallation sources will continue to remain inferior to CW reactor sources (also in terms of cost/performance ratio) in those applications which currently are best performed at the leading CW sources. These applications notably include most of thermal neutron and virtually all of cold neutron diffraction and spectroscopy. For the first time in spallation history, maximized intensity coupled moderators have been installed at LANSCE, and this opens up opportunities for achieving by now unprecedented instrument performances at spallation sources, in particular in cold neutron spectroscopy, such TOF-BS.

2. TOF-Backscattering with an optional pulse-shaping chopper.

The aim of our proposed improvement of the standard TOf-BS technique (IRIS) is to provide better and easily tunable resolution at best possible intensity conditions and unrestricted q range. This flexibility will largely enhance the instrumental capability in many respects. For example a weak very sharp structure in the spectrum can be lost in the instrumental background if looked at with insufficient resolution.

Compared to CW backscattering instruments existing TOF-BS spectrometers like IRIS at ISIS [1] are characterized by a large dynamic range due to the inverted geometry (e.g. from -0.2 to 3.5 meV) and a moderate energy resolution of 15 μeV. For example IN10 (ILL) offers ~ 1μeV energy resolution at a dynamic scan width of not more than ± 30 μeV, although it has been proposed to enhance dynamic range to 500 μeV by scanning the temperature of the monochromator crystal [2]. Using bent crystal elements also allows adjusting somewhat the resolution [3]. Let us note that the large dynamic scan range of the pulsed source instruments is not always a real advantage. On the one hand side, it allows one to investigate large energy transfers with the basic good resolution (which on CW sources can only be achieved by scanning the temperature of the monochromator or by the rather cumbersome way using a monochromator crystal different from the analyzer.) On the other hand, often there are no sharp structures requiring high resolution distributed over a broad energy range, so much of the, at pulsed sources little adjustable, broad scan delivers no useful information.

The scheme of a TOF-BS spectrometer with an optional fast pulse-shaping chopper is shown in Fig. 1. The Si analyzer crystals are assumed to cover part of the analyzer solid angle and another part is covered by graphite crystals, quite similarly to the manner mica and graphite are disposed in IRIS on two opposite sides of the scattering chamber.

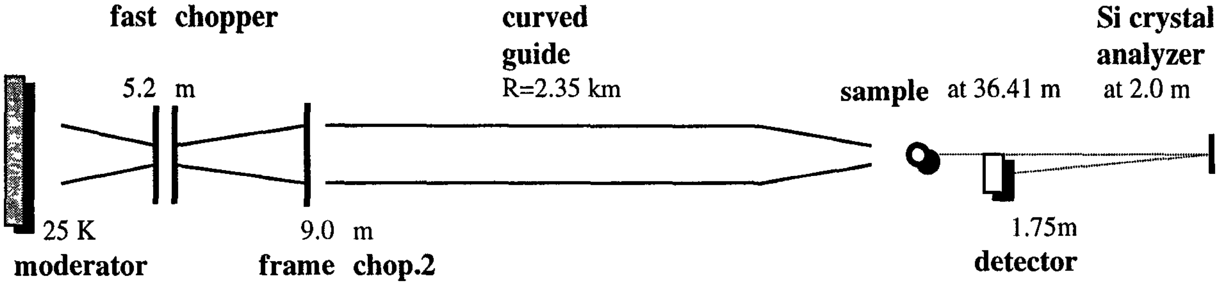

Figure 1. Layout of a pulsed source backscattering instrument with an optional fast chopper at 5.2 m from the moderator. The other distances essentially correspond to that of IRIS.

3. Instrument performance evaluated by Monte Carlo simulation

The Monte-Carlo simulation technique we have developed for evaluating experiments at IRIS has been described elsewhere in detail. Compared to IRIS, the basic difference in the high-resolution operation mode is that the incoming neutron pulse length is determined by the fast chopper. We have assumed a 250 Hz revolution disc chopper device with two counter-rotating discs producing 23.5 μs pulses. An 'eye-of-the needle' convergent + divergent $3\theta_{Ni}$ supermirror guide combination [5] was assumed to focus the neutrons from the moderator on the fast chopper window, in order to reduce the beam width at the chopper, i.e. to achieve a shorter pulse length. Note that a Fermi type chopper could also be envisaged instead of the disc chopper, since only a narrow wavelength band is to be transmitted simultaneously. The moderator pulse was assumed to display the 150 μs FWHM pulse shape corresponding to what is expected at LANSCE for a partially coupled liquid H_2 moderator. (Fig.2). The disc chopper at 9 m serves to eliminate frame overlap from consecutive pulses. It is a standard feature of the IRIS type design. In order to improve the angular resolution for the scattered beam the spherically focussing Si(111) analyzer crystal arrangement was assumed to be at 2 m from the sample. This extension of the total flight path has little effect either on the TOF resolution or on the analyzer energy resolution.

The cylindrical sample size ($r = 1$ cm, $h = 3$ cm) considered is small enough to avoid reduction of resolution due to TOF path differences. The analyzer was assumed to consist of 0.5×0.5 cm flat elements, in order to achieve perfect focussing to the detector. The spot size on the detector determines the angular resolution. In the current simulation we have only concentrated on the energy resolution, which is fairly well decoupled from the angular or q resolution. The sample scattering function used in the calculations was independent of momentum transfers. A single scattering angle, 140° was evaluated, at which angle the path differences in the sample is close to the worse case maximum. The sample absorption was set to a negligible level.

Some results of the simulation calculations are shown in the next two figures. In Fig 3 the instrumental resolution is illustrated by the calculated instrumental response for a model quasielastic Lorentzian line with 1μeV FWHM. The "measured" line can be fitted by a Lorentzian with 2.9 μeV FWHM, thus the instrumental energy resolution amounts to about 2 μeV FWHM.

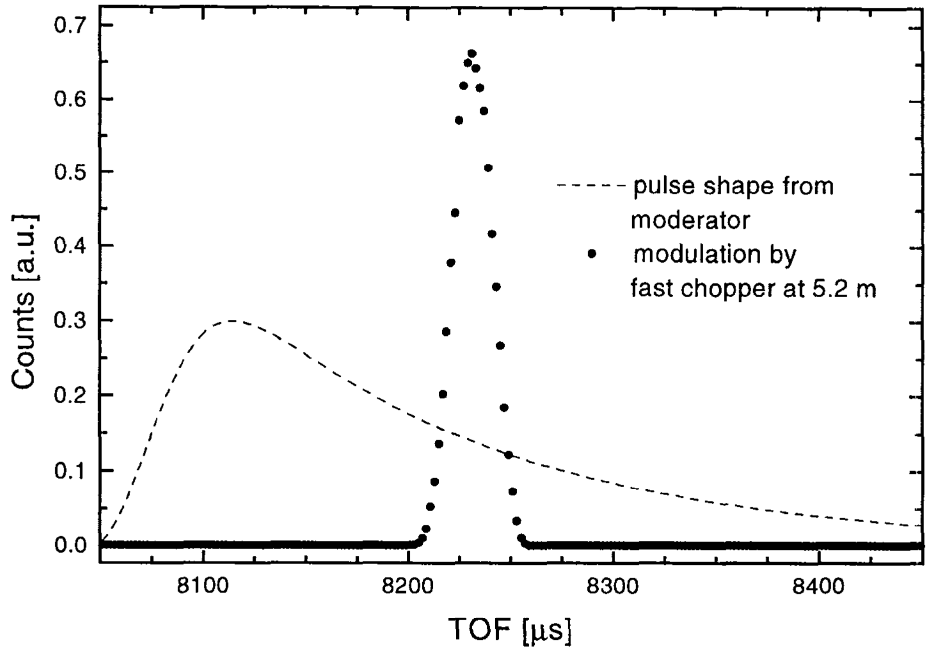

Figure 2. Comparison of the partially coupled moderator pulse shape (expected at LANSCE, analytic approximation) and the fast double disc chopper pulse shape (simulation).

Due to the finite distance, determined by the thickness of the bulk shielding, between the moderator and the fast pulse-shaping chopper, the moderator – chopper system also act as a monochromator, i.e. only neutrons in a narrow neutron energy band width pass the chopper. This band determines the scan width in the chopper mode of operation, which turns out to be rather close to the those achieved on CW source high resolution instruments, as discussed above. In order to explore this scan width we have calculated the instrumental response to a series of inelastic lines separated by 10 μeV. The results in Fig. 4 show indeed that we can efficiently simultaneously explore an energy interval of about 90 μeV, which is very small compared with scan width of the instrument in the low resolution (15 μeV) conventional IRIS type configuration with the fast chopper removed (or stopped in the open position, a standard feature of state of the art disc choppers). Here again, as discussed above in connection with the similarly narrow scan width of the CW source backscattering instruments, this simultaneously explorable narrow energy window will rarely mean a particular handicap. Typically one will be interested in zooming in with high resolution to a particular structure in the spectrum only. By adjusting the phasing of the fast chopper, one can easily position the high resolution scan window to any part of the broad energy range normally accessible in the low resolution configuration, a clear advantage compared to CW instruments.

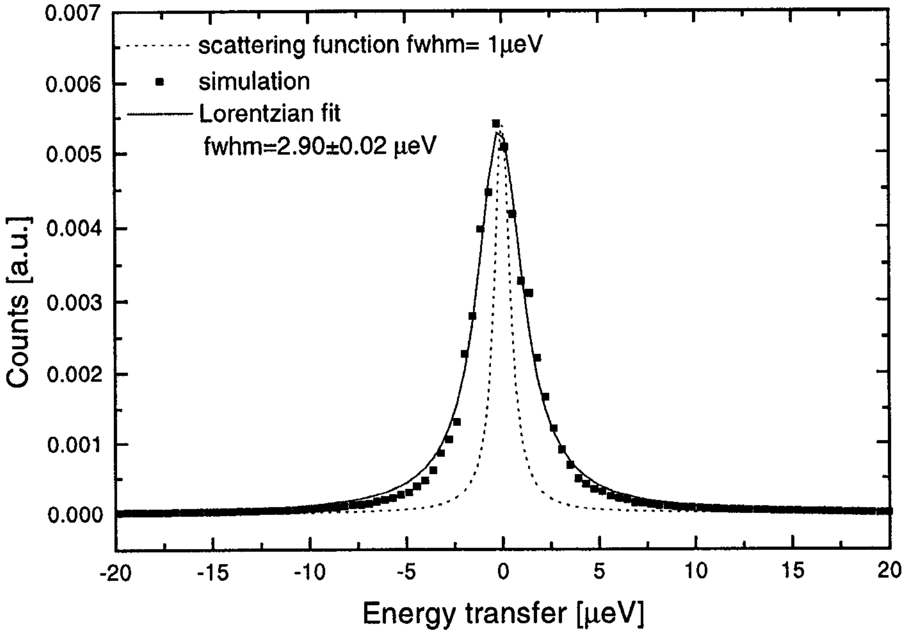

Figure 3. Evaluation of the instrumental resolution: simulated data points for a Lorentzian quasielastic line of 1 μeV full width (dotted line). The solid line is a Lorentzian fir to the simulated data.

The scattered beam intensity relative to the best similar resolution CW source instruments has not been evaluated in this simulation. A rough analytic estimate shows that assuming the planned flux at LANSCE after the upgrade the high resolution mode of operation considered here would offer comparable counting rates for equal analyzer solid angle and 2 times less resolution than the recently built IN16 at ILL. The narrow scan width (Fig. 4.) means an effective data collection duty factor of about 3 %, compared to the 50 % duty factor of the CW spectrometers (background chopper). This is partially compensated by the about 4 times higher peak flux and by the fact that the resolution cannot be traded for intensity on IN16 beyond 1 μeV.

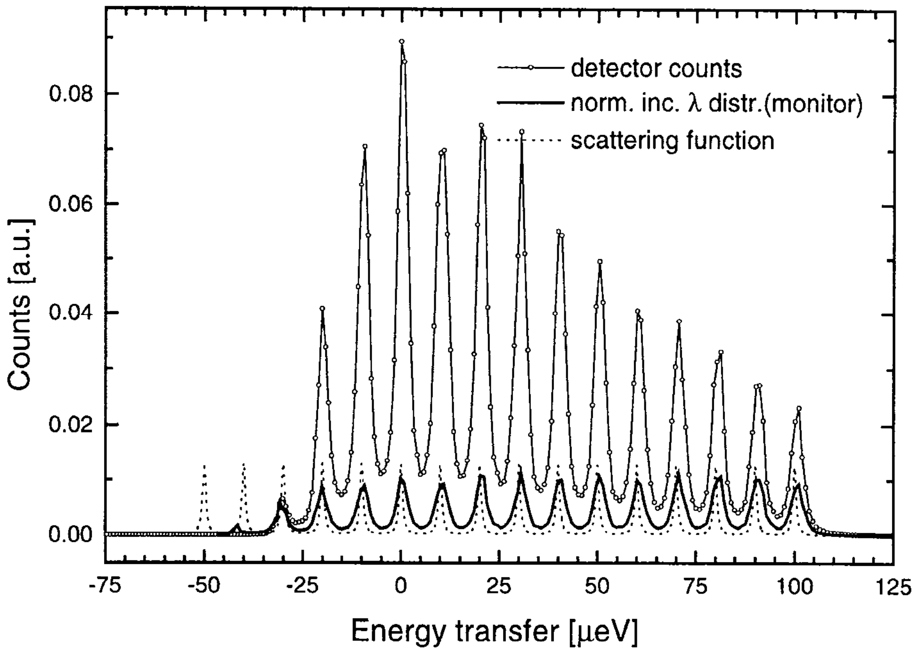

Figure 4. Evaluation of the simultaneously explored energy window: the instrumental response to a series of inelastic lines separated by 10 μeV. The dashed line shows is the model scattering function, the points are the simulated data and the lower solid curve is the "measured" spectrum normalized to the moderator pulse shape in Fig. 2.

4. Conclusion

The pulse-shaping fast chopper and Si crystal analyzer option can very efficiently enhance the global performance of a standard IRIS type pulsed source backscattering spectrometer by offering the possibility to zoom in to parts of the studied spectra with an about 7 times better resolution. In this high-resolution mode of operation a spectrometer at a source like LANSCE will provide comparable intensities to the best existing μeV resolution reactor source instruments.

References

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