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New capabilities in spectroscopy on pulsed sources: adjustable pulse repetition rate, resolution and line shape

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Abstract

Spectroscopy with cold neutrons is one of the most important areas of current superiority of reactor based instruments over those at spallation sources. This is particularly due to the capability of continuous source time-of-flight spectrometers to use instrumental parameters optimally adapted for best data collection rate in each experiment. These parameters include the pulse repetition rate and the length of the pulses to achieve optimal balance between resolution and intensity. In addition, the disc chopper systems used provide perfect symmetrical line shapes with no tails and low background. We present a set of novel techniques making up the IN500 project at Los Alamos, which is based on the combined use of extended pulse length, coupled moderator, disc chopper system and advanced neutron optical beam delivery. This development will enable Lujan center to surpass the best reactor sources in cold neutron spectroscopy by realizing for the first time all of the above key capabilities of steady state instruments on a pulsed spallation source.

1. *Introduction*

The major part of neutron scattering research is today performed on steady state reactor sources. However, the next generation of neutron sources will be pulsed. In this new situation we face the challenge to develop novel neutron scattering techniques, which will make all instruments at pulsed sources competitive with reactor sources instruments, even those which are not competitive today. Examples of such techniques is the subject of the IN500 project at LANSCE/Los Alamos, to develop high performance cold neutron time-of-flight (TOF) spectroscopy specifically for pulsed sources, while offering all the capabilities to optimally adjust the instrumental parameters to the experiment which made reactor based instruments so much superior in the past. The project takes advantage of the coupled liquid H_2 moderator recently installed at Lujan Center. The new moderator provides longer pulses (FWHM ~ 300 μsec) and higher flux (~ 3 times that of ILL in peak and ~ 3 % of it in time average). Further innovative features used in the project include the more effective use of the pulsed neutron flux by Repetition Rate Multiplication, reduction of losses in the beam delivery system (Ballistic Guide) and pulse shaping in order to improve the resolution and the signal to noise ratio and to optimize the flux according to the experimental requirements.

2. Enhanced efficiency by Repetition Rate Multiplication

One major source of reduced data collection efficiency in neutron scattering spectroscopy at pulsed sources is the large difference between the repetition rate of the source and the repetition rate required by the instrument. The optimal repetition rate of TOF spectrometers is determined by the time needed to analyse the scattered neutron spectra over the flight path of 2 – 6 m in the secondary spectrometer, and it is in the range 100-500 Hz. In contrast, the repetition rate of existing and planned pulsed spallation sources is 10-60 Hz. Thus the conventional principle of working with only one monochromatic wavelength per pulse only allows us 10-50% efficient use the available data collection time. The Repetition Rate Multiplication (RRM) principle [1] helps to enhance efficiency by delivering on the sample several neutron pulses with several monochromatic wavelengths from each source pulse, instead of a single pulse of a given wavelength. The repetition rate of the instrument thus becomes independent of the source repetition rate and it will be defined by the requirements of the experiments, similarly to the spectrometers on reactor sources.

In the IN500 project Repetition Rate Multiplication will be realized by a disc chopper system (Fig.1) combining features of that of IN5 at ILL or NEAT at HMI with those of conventional wavelength band choppers at spallation sources. The slow choppers #1 and #2 rotating with the same frequency as the source (20 Hz) define a broad wavelength band, which is later cut into a set of monochromatic pulses by fast choppers #3 and #6, also defining the primary and secondary resolution of the instrument. While slow choppers are designed to avoid overlap between neutrons coming from different source pulses, fast choppers are aimed to avoid the overlap between neutrons of different wavelengths coming from the same source pulse. In particular, chopper #4 eliminates spurious contributions coming from the long time tail of the source pulse (up to 4 ms) and "leaking" trough the resolution defining choppers #3 and #6. The function of chopper #5, not shown in Fig. 1, is to suppress every second, third or fourth pulse from the basic 240 Hz pulse rate at the sample in order to prevent the frame overlap of scattered neutrons in the secondary spectrometer between the sample and the detectors.

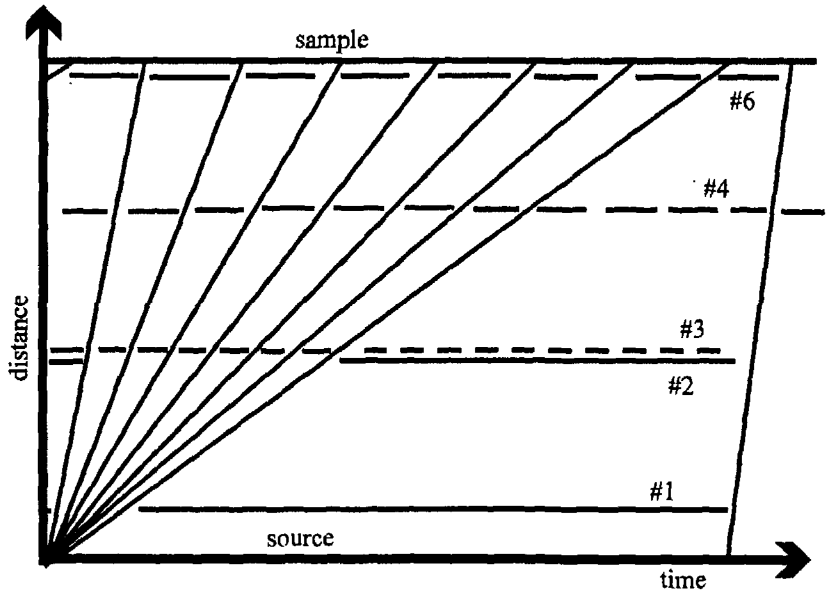

Fig. 1. Principle of Repetition Rate Multiplication as realized by a disc chopper system. The source to sample distance in the IN500 project is 63 m, and time between source pulses 50 ms.

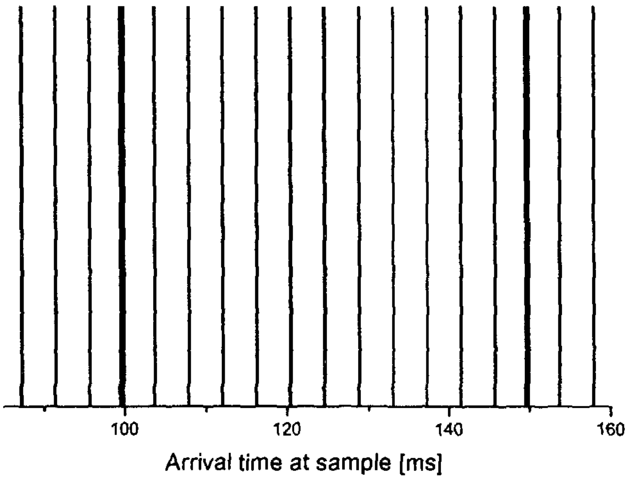

Fig. 2. Neutron pulses arriving to the sample on IN500 as a function of time in 12 fold Repetition Rate Multiplication operation at the 20 Hz Lujan Center. The 240 Hz pulses between 105 and 147 ms are the useful pulses emanating from the source pulse at t=0. Pulses around 99 and 149 ms overlap with a pulse from the previous or the subsequent source pulse, respectively. The figure indicates total duration of pulses, not the true pulse shape.

The IN500 chopper system was designed and optimized by the new approach of "wavelength filtering", proposed by one of the authors (FM). The main principle is to divide the chopper system into from each other independent sub-units of lower numbers of choppers. First, the transmission is studied for such sub-units alone, and an upper limit of the transmission of the total system is built as an overlap between the transmissions of the sub-units. This overlap was then maximized by shifting the opening time pattern of the sub-units relative to each other (phasing). Fig. 2 shows a pulse sequence on the sample for the complete chopper system, with no pulses suppressed by chopper #5. The first (shortest wavelength) and the last (longest wavelength) pulses from subsequent source pulses overlap (double pulse in the figure) and will be excluded from data analysis. All the other pulses are cleanly separated, and all possible parasitic pulses (not shown) have wavelengths above 90 Å, and therefore negligible intensities. The wavelength difference between subsequent pulses from one source pulse is 0.2646 Å, and the 2.91 Å band between the shortest and longest wavelengths can be freely chosen between some 2 and 20 Å.

3. Adjustable resolution

The pulse shapes at spallation sources have a strongly asymmetric form resulting in asymmetric instrumental resolution functions (Fig. 3). Thus, the signal-to-background ratio close to the elastic signal on instruments at pulsed spallation sources is usually worse than that at reactor sources. Furthermore, different experimental needs lead to the requirement of a tunable (flexible) instrumental resolution, in order to be able to trade resolution for intensity. To adjust the resolution according to the experimental requirements, in the IN500 project we phase one of the resolution defining choppers, #3 to the source in a manner to cut a part of the tail of the pulse. By shifting in time the chopper phase we can cut more or less of the trailing

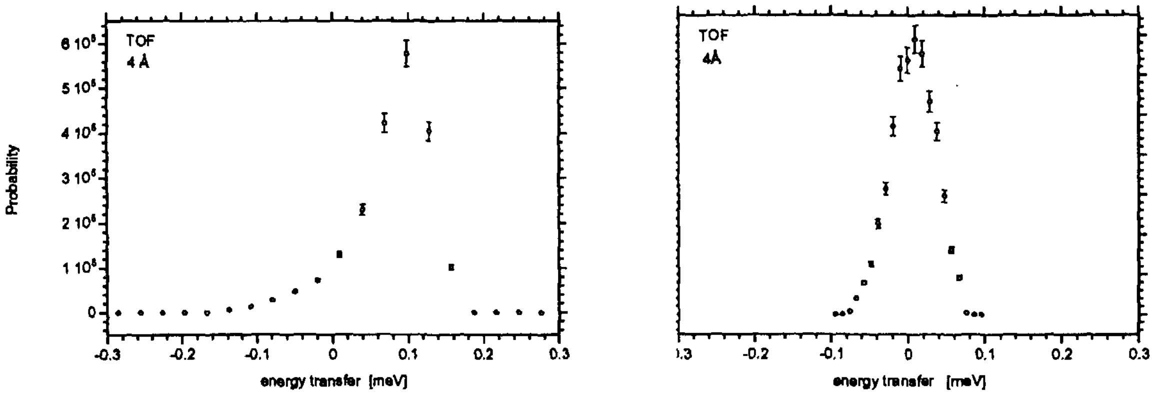

Fig. 3. Monte-Carlo simulated elastic line shapes for IN500 with no pulse tail cutting (left) and with chopper #3 phased to cut the coupled cold moderator pulse at Lujan center at 0.5 ms.

edge of the source pulse while taking full advantage of its sharp rising edge. Our calculations (Fig.3.) show that after the pulse shaping by chopper #3 the resolution function has a pretty symmetric shape and at the same time we can achieve resolutions even better than that of IN5 at ILL, and comparable to that of the backscattering spectrometer IRIS at ISIS (Fig. 4). Variable secondary spectrometer resolution is achieved by the capability of selecting different slit widths on chopper #6, which actually is a counter-rotating pair of fast disc choppers.

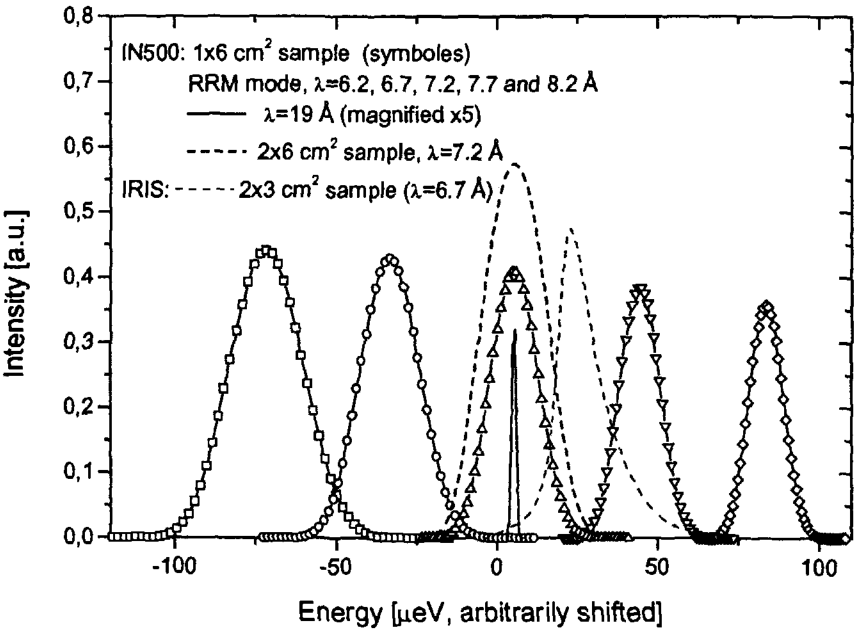

Fig. 4. Calculated elastic line shapes for the best resolution configuration of IN500. Chopper #3 cuts the source pulse to 220 μs FWHM length, chopper pair #6 is set to 20 μs FWHM. All pulses are centered at 0 energy and arbitrarily shifted for visibility. The symbols correspond to retaining via chopper #5 each second pulse only from a sequence similar to that in Fig. 2. The elastic response of IRIS, included for comparison, is approximately to scale in intensity.

4.Low losses beam delivery by ballistic neutron guide

RRM works the more efficiently the larger is the distance between the source and the sample, i.e. the smaller the difference is between the wavelengths of subsequent pulses on the sample from the same source pulse. In the case of IN500 this distance is 63m. Intensity losses by the beam transport over such long distances are mainly caused by less then perfect reflectivity of the coatings used in neutron guides. Thus to reduce the losses we need to decrease the number of reflections, which can be achieved by using a so called Ballistic Guide [1]. The ballistic guide includes three parts: a Ni coated neutron guide with large cross section over most of the length and one diverging and one converging supermirror coated section coupling the Ni-guide to the moderator and to the sample, respectively. The diverging guide leads to a more parallel neutron beam, which in the large cross section of the Ni guide undergoes drastically reduced number of reflections. Based on the results of our simulation study we expect nearly an order of magnitude better performance for the ballistic guide compared to the beam transport efficiency in a conventional supermirror coated guide [2].

5. Summary

The combined effect of the innovations to be implemented in the IN500 project, i.e. the use of a) a high intensity coupled moderator, b) a disc chopper system capable to simultaneously realize multiplied pulse repetition rates on the sample, perfect symmetric line shape and variable resolution and c) a reduced loss neutron guide system, will provide about 30 times higher flux on the sample at the designed 160 kW power of Lujan center at Los Alamos than the most powerful cold neutron spectrometers in existence today, IN5 at ILL and NEAT at HMI. (The currently started reconstruction of IN5 is expected to bring a gain of a factor of 8 – 10 in the future.) Furthermore, as test experiments at HMI have shown [3], advanced TOF techniques make the TOF approach comparable in efficiency to the triple axis method on the same continuos source, even for constant **q** spectroscopy in single crystals. Consequently, the IN500 project will not only deliver new capabilities in conventional applications of cold neutron TOF spectroscopy, but it will also provide for the first time a spallation source instrument competitive with top performance cold neutron triple axis spectroscopy for the study of excitations in single crystals.

References

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