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Monte-Carlo simulations of a high-resolution inverse geometry spectrometer on the SNS - Long Wavelength Target Station

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Abstract. Using the Monte-Carlo simulation program McStas, we present the design principles of the proposed high-resolution inverse geometry spectrometer on the SNS - Long Wavelength Target Station (LWTS). The LWTS will provide the high flux of long wavelength neutrons at the requisite pulse rate required by the spectrometer design. The resolution of this spectrometer lies between that routinely achieved by spin echo techniques and the design goal of the high power target station backscattering spectrometer. Covering this niche in energy resolution will allow systematic studies over the large dynamic range required by many disciplines, such as protein dynamics.

1. Description of the instrument – The basic design

The concept of the inverse geometry spectrometer came about with the plans to build a Long Wavelength Target Station (LWTS) at SNS [1], which will provide high flux of long wavelength neutrons. The actual instrument design employs mica analyzers close to backscattering geometry (final neutron wavelength of 20 Å), with an extremely high-energy resolution ($\delta\omega \leq 0.2$ μeV FWHM, elastic).
In order to optimize the layout of individual components and to estimate the instrument performance, the Monte-Carlo simulation program McStas [2], developed at Risø National Laboratory, has been used. McStas offers a general framework to compose a virtual neutron scattering instrument and supports both reactors and spallation sources.
Consider that the uncertainty in the energy transfer for an inverted-geometry spectrometer using crystal analyzers can be separated into a term dependent on the primary spectrometer ($\delta\omega_P$, components before the sample) and on a term dependent on the secondary spectrometer ($\delta\omega_S$, components after and including the sample). And taking the approximation that the terms are independent and that the uncertainties add in quadrature the energy resolution function is given by [3],

$$\delta\omega = \sqrt{\delta\omega_P^2 + \delta\omega_S^2} \qquad 1$$

Where,

$$\delta\omega_{\mathrm{P}} = 2E_i \left(\left(\frac{\delta L_i}{L_i} \right)^2 + \left(\frac{\delta t_0}{t_i} \right)^2 \right)^{\frac{1}{2}} \qquad 2$$

And

$$\delta\omega_S = 2\left(E_i^2 \left(\frac{\delta t_f}{t_i} \right)^2 + E_f^2 \left[(\cot(\theta_B)\delta\theta_B)^2 + \left(\frac{\delta d}{d} \right)^2 \right] \right)^{\frac{1}{2}} \qquad 3$$

Where
E_i is the incident neutron energy,
L_i is the moderator-sample distance,
t_i is the incident neutron flight time,
t_0 is the emission time of the neutron from the moderator and
t_f, is the time for the neutron of known final energy to travel from the sample to analyzer to detector.
On a crystal analyzer spectrometer, the final neutron energy, E_f, is fixed by Bragg reflection from the analyzer crystals.
The first term in Equation 2 is small compared to the second, and therefore the contribution from the primary spectrometer to the resolution arises from the moderator pulse width (δt_0) at a given neutron energy. On the other hand, the contribution from the secondary spectrometer (Equation 3) represents uncertainty in the lattice parameter (δd) of the crystal analyzers and the uncertainty of the Bragg angle ($\delta\theta_B$). $\delta\theta_B$ has contributions both form the analyzer crystal mosaic and the sample dimensions.
Traditionally, the resolution contributions from the primary and secondary spectrometers are matched in an effort to optimize the count rate in the detectors for a given resolution. The decoupled poisoned solid methane moderator at LWTS generates a pulse with a width of 90 μsec for λ = 20 Å. For a neutron λ of 20 Å the energy reflected from the (002) planes of mica is 0.2045 meV. In order to achieve the timing resolution necessary for the desired δω, the primary flight path of the spectrometer a long initial guide section around 63 m from moderator to sample is required. For many reasons it is desirable to design the instrument with the analyzers slightly out of backscattering. In fact, this component of the resolution, $\cot(\theta_B)\delta\theta_B$, can be relaxed from exact backscattering, without modifying the overall resolution significantly [4]. A reasonable choice is based on sample/detector geometry to opt for a Bragg angle of 87.5˚.
In contrast to spectrometres such as IRIS with lower resolution requirements, in this particular case the sample size can easily dominate the first and second terms in Equation 3. Restricting the sample size is not an issue in case where only limited amount of sample are available. However, when sufficient sample is avaiable, a restricted beam size lowers the neutron flux into the detector. Optimization of the secondary spectrometer requires to keep the first term of Equation 3 small compared to the second. Constraining the design to a 2 m sample-analyzer flight path, leads to an optimazed sample size of 2 x 2 cm^2 and a sample-size contribution of 0.41˚. The total contribution of the sample size to Equation 3 is 163 neV (to be added in quadrature to the $\delta\theta_B$ contribution from the the analyzer mosaic).
It is also important to understand the contributions to the Q-resolution for energy transfers near the elastic peak. In this case, the momentum transfer is given by,

$$Q = \frac{4\pi \sin(\frac{\phi}{2})}{\lambda_f} \qquad 4$$

where ϕ is the angle between the incident neutron beam and the scattered beam. Differentiating the previous equation and considering that the uncertainty in λ_f is small, the uncertainty in Q is given by:

$$\delta Q = \frac{4\pi}{\lambda_f} \cos(\frac{\phi}{2}) \frac{\delta\phi}{2} \qquad 5$$

The contributions to $\delta\phi$ are the incident beam divergence $\delta\phi_i$, the contribution from sample size $\delta\phi_S$ and the acceptance of the analyzer $\delta\phi_A$.

2. Description of the instrument – Details of the spectrometer design

The backscattering spectrometer tank is a 2 m diameter vacuum vessel as shown in Figure 1. In order to eliminate frame overlap at the sample position a disk chopper is located directly outside the target station. The bandwidth chopper gives a wavelength band of 6.219Å delivered to the sample at 63.36 meters from the moderator. This wave length band provides a range of energy transfers for the mica (002) reflection of ±60μeV. The performance characteristic of the instrument for near elastic scattering is as listed on Table I.

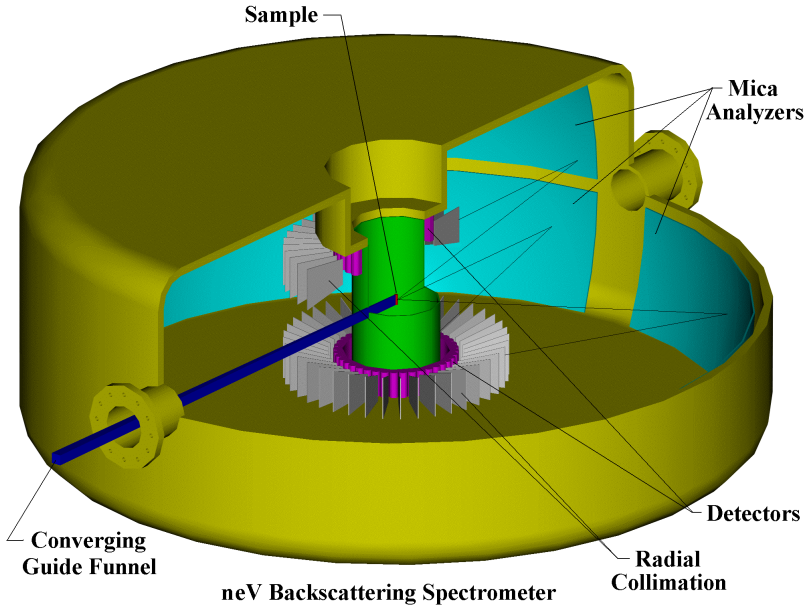

Figure 1 – The layout of the neV-backscattering guide system at the LWTS at SNS.

Table I – Spectrometer performance for near elastic scattering.

Analyzer crystal	λ_f (Å)	$\Delta\lambda_f$ (Å)	ω-range (μeV)	δω (fwhm) (μeV)	Q-range (Å^{-1})	δ Q (fwhm) (Å^{-1})
Mica (002)	20	6.219	-60 to 60	0.215	0.05 to 0.6	0.015 to 0.002
Mica (004)	10	6.219	-420 to 420	1.14	0.1 to 1.2	0.03 to 0.004

Preliminary guide optimization was carried out by iteration of a Monte Carlo simulation. A curved guide 30 meters long with radius of curvature of 1km giving a characteristic wavelength of 7.9 Å with a critical angle equal to that of natural nickel was selected. The guide begins at 8.34 meter from the moderator accepting 20 Å neutrons with 0.5˚ divergence. The straight guide is made from sections of 1 meter each, with a total length of 18.77 meters. The guide cross-section is 6 cm x 6 cm ending in a 6 meter long natural nickel funnel that stops 25 cm from the sample with exit dimension of 2 cm x 2 cm. Total guide gains (ratio of neutrons on the sample with and without a guide) were estimated at 360 for λ = 20Å. A description of the guide components is given on Table II, and the scattering chamber design is illustrated in Figure 2.

Table II - Description of the guide components

Component	**Description**	**Characteristic**
Moderator	Decoupled, 30mm poisoned solid methane	δt_0 = 90 μsec for λ = 20 Å
Analyzer Crystal	Bragg Angle	87.5 deg
	d-spacing	mica (002)
Incident Flight Path	20 cm (H) x 15 cm (V) Guide/Funnel	63.36 m from moderator to sample
Guide (cross section 6 cm)	Moderator-Guide Distance	8.34m
	Curved Guide Length	30m
	Straight Guide Length	18.77m
	Guide Funnel Length	6 m (natural Ni)
	End of Funnel - Sample Distance	0.25m
Sample	Geometry varied	2 x 2 cm^2 cross section of neutron beam
	Sample-analyzer distance	2m

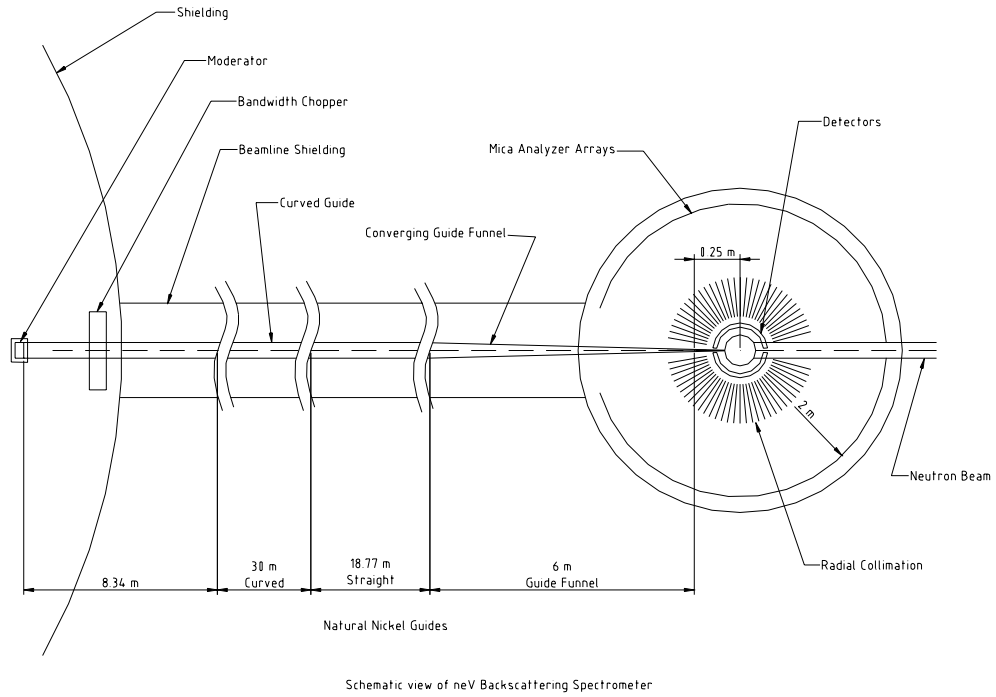

Figure 2 – Schematic view of the neV-backscattering at the LWTS at SNS.

The mica analyzers are located plus and minus 20˚ out of the scattering plane covering scattering angles from 5˚ to 160˚, 2 meters from the sample, and have a mosaic spread estimated to be about 0.25˚ (fwhm). The detectors are approximately 175 cm from the analyzer crystals.
The peak count rate is expected to occur at the elastic peak. A typical case is when the total sample scattering is 10% of the incident beam flux. If elastic scattering dominates, the number of neutrons scattered into the elastic peak is given by

$$N_S = F \times s \times \omega_R \times 0.1 \qquad 6$$

Where F is the expected flux on the sample, s is the sample size and ω_R is the resolution width of the primary spectrometer. For the mica high-resolution backscattering instrument at LWTS F = 3.5$10^4$n/cm^2-sec-μeV (2MW, with a guide gain of 360), s is 4 cm^2 and ω_R is 0.14 μeV, making N_S = 1960 n/sec.
Each analyzer segment intercepts 1.85 ster of solid angle. Allowing a 20% loss for imperfect crystal reflectivity and loss due to mosaic spread, the number of neutrons intercepted by the detectors, F_D, is

$$F_D = \frac{3.7}{4\pi} \times N_S \times 0.8 = 462 \text{ n/sec} \qquad 7$$

An important figure of merit that should be estimated is the time required to obtain counts in the peak channel of the elastic peak for the 10% scattering sample:

$$t = P_T \times \frac{1}{F_D} \times N_Q \times \frac{N_R}{2} \qquad 8$$

Where P_T is the desired number of counts, N_Q is the total number of single Q-point that gets summed into the detector and equal to 10 in this case, N_R is the number of bins across the elastic peak into which counts are stored, with a typical value of 20. The factor 2 corrects for the approximately triangular shape of the resolution function. As an example, the time required to obtain 4000 counts in the peak time channel is approximately 15 minutes.
A similar analysis done for the performance of this instrument if it is built at the HPTS (high power target station) at SNS shows a decrease in the performance of a factor of 4 in flux on sample. In addition, pulse suppression choppers would be required to eliminate intervening pulses with an attendant uncertainty in background.

3. Monte Carlo Resolution Function

Of most interest is the resolution at the elastic peak. The simulation was carried out with a cylindrical shell vanadium sample that only scattered elastically. The sample was a hollow cylinder with an inner radius of 1.85 cm, an outer radius of 2.0 cm and was 2 cm high. For this calculation 108 crystal analyzers were used covering 3˚ in the scattering plane and 20˚ in the horizontal plane. The crystals had dimensions approximately 2 cm x 2 cm. Counts were collected using 3 position sensitive detectors, with 15 position channels each, (1 cm long channels along the length of the tube and 15 cm active length), infinitely thin, and 1 cm wide. The detectors were binned at 10 μsec time channels making possible a good line-shape analysis.

For the current target design, the moderator was modeled as a combination of Gaussians. As we can see on Figure 3, due to the tail on the moderator the resolution function is slightly asymmetric.

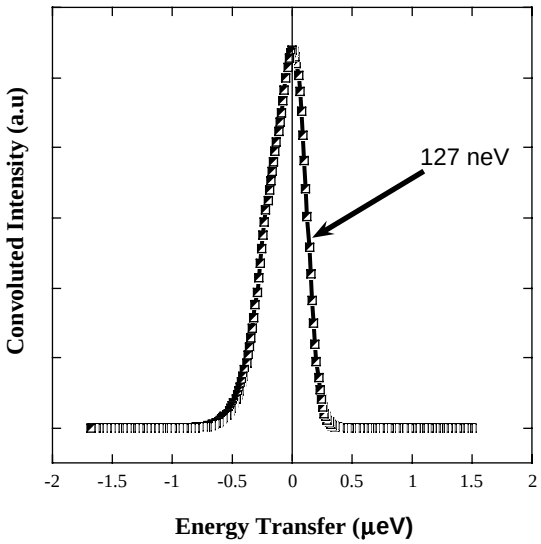

Figure 3 – Resolution function at the elastic peak.

Improvements to the current design could include changing the moderator poison depth to a shallower position. This choice would improve the resolution but at a loss of flux on sample. A softer constraint on the instrument design is the initial flight path length. Because of the high transmission of the natural Ni guide, this distance can be increased without significantly changing the instantaneous flux on sample. Its sole effect would be to decrease the range of energy transfers accessible in a single frame measurement. This option could improve the resolution of the instrument by improving the resolution of the primary spectrometer. Other considerations include moving the spectrometer to a coupled moderator, and use a pulse-shaping chopper to modify the long time tail of the moderator pulse. However due to the large bandwidth necessary (6.219Å) for the performance of the instrument, this solution may not be viable. Another possibility is the use of a Drabkin flipper, [5] where the basic idea is to create a resonance condition such that only neutrons having two selected parameter values (in time and in wavelength) will be transmitted. Neutrons that do not fulfill both conditions, for example those neutrons from the moderator tail, will not be reflected by the second mirror. After transmission through the energy filter, the wavelength-time relation will be much sharper than before. Another useful application of the device is that it will filter out the steady background of delayed neutrons, which are constantly emitted from the target or from activated shielding. However, this requires the use of a polarized neutron beam and a loss in neutron flux on sample of at least a factor of two.

4. Optimization of long-wavelength analyzers

Mica are alumino-silicate minerals with a sheet structure having two layers of silicate tetrahedra arranged between a layer of hydrated metal-oxide octahedra, existing in different species such as muscovite, annite, phlogopite, fluoro-phlogopite and biotite. Slabs of single crystalline mica are of interest as a cold-neutron monochromators or analyzers in high-resolution spectrometers due to their large lattice spacing (about 10 Å). Recent investigations

[6] of synthetic fluorinated mica, fluoro-phlogopite $K_2Mg_6(AlSi_3O_{10})_2F_4$, shows strong (002) and (006) reflections and a weak (004) reflection with very low thermal diffuse scattering. Natural phlogopite, $K_2Mg_6(AlSi_3O_{10})_2(OH)_4$, show all reflections consistently strong with higher backgrounds. Fluorinated mica has the following unique characteristics: high chemical stability, excellent reflectivity, outgasing-free at high temperature in vacuum, excellent electrical insulation, high heat endurance (up to 1100 °C), non-radioactive background, highly flexible and cleavable, which are much superior to that of natural mica. In addition, large fluorinated mica crystals of high quality can be grown by a Bridgman-Stockbarger method [7]. Given the lower background due to greatly reduced incoherent scattering, it is reasonable, despite the greater price, to consider fluoro-phlogopite as an option. However, it is clear that optimization of the crystal analyzers is crucial to the operation of the spectrometer. Parameters such as neutron reflecting properties [8] and ideal crystal thickness must be fully explored.

5. The scientific impact of the mica backscattering instrument at LWTS

The LWTS will provide the high flux of long wavelength neutrons at the requisite pulse rate required by the spectrometer design. The proposed 200 neV spectrometer (using the mica (002) reflection) offers a remarkable Q-range 0.05 $Å^{-1} \leq Q \leq 0.6$ $Å^{-1}$, with a high Q resolution of 0.002 $Å^{-1} < \delta Q < 0.015$ $Å^{-1}$ and excellent dynamic range of -60 μeV $< \omega <$ 60 μeV. Options include using higher order reflections to extend the ranges of both energy and momentum transfer. The resolution of this spectrometer lies between that routinely achieved by neutron spin echo techniques and the design goal of the high power target station backscattering spectrometer. Covering this niche in energy resolution will allow systematic studies over the large dynamic ranges of energy transfer required by many disciplines. The complete set of SNS spectrometers, including the proposed LWTS neV instrument, will open unprecedented opportunities in the areas of chemical and biomolecular dynamics. Such studies often require systematic investigation of many similar molecules under slightly different conditions, requiring a large range of energy/timing resolutions for optimum study.

References

[1] SNS Long Wavelength Target Station Conceptual Design - NSF Proposal P-00106
[2] K. Lefmann and K. Nilesen, Neutron News **10/3** (1999) 20.
[3] K.W. Herwig, Oak Rigde National Laboratory ES-1.1.8.4-6017-RE-A-00 (1999), and private communication.
[4] C.J. Carlile and M.A. Adams, Physica B **182** (1992) 431.
[5] Frank Klose, SNS Design Criteria for the SNS Instrument Systems Magnetism Reflectometer
[6] P. Allenspach and D. Engberg, PSI - Focus Progress Report (1998).
[7] Pengdi Han, H. C. Materials Corporation, Private Communication (1999).
[8] M.L. Crow, Physica B **241-243** (1998) 110.