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Doppler-Musical Instrument

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We propose a possible ultra-high energy resolution backscattering spectrometer optimized to spallation neutron source. A combination of multi monochromator crystal and Doppler drive provides considerable neutron flux, together with the reasonable energy range $-30 < E < 30$ μeV, even when the ultra-high energy resolution of $\Delta E \sim 0.03$ μeV is attained.

1. Introduction

Neutron backscattering is one of the most important techniques to enable ultra-high energy resolution neutron spectroscopy [1]. The basic idea of backscattering is to use a perfect single crystal with $\theta = 90°$ Bragg reflections. The energy resolution, obtained with the backscattering condition, is given as,

$$\frac{\Delta E}{E} = 2\frac{\Delta k}{k} \simeq 2\left(\frac{\Delta\tau}{\tau} + \frac{(\Delta\alpha)^2}{8}\right), \quad (1)$$

where $(\Delta\tau/\tau)$ is the intrinsic line width due to primary extinction. Since Eq. 1 does not include a first order term of $\Delta\alpha$ (neutron beam divergence), the energy resolution becomes insensitive to the beam divergence, or in other words, large beam divergence can be acceptable. As concerns the first term in Eq. 1, $(\Delta\tau/\tau)$ can be as small as 1.86×10^{-5} or 0.157×10^{-5} for Si(111) or GaAs(200), which results in the energy resolution of $\Delta E \sim 0.077$ or 0.008 μeV, for perfectly collimated beam [2]. Thus, the ultra-high energy resolution spectrometer can be realized, in principle.

To obtain a very-high energy resolution, it is crucial to use the backscattering method for both the monochromator and analyzer. Thus, to date backscattering spectrometers are constructed at reactor-based continuous neutron sources, such as IN16 at ILL. For the spallation (or pulsed) neutron source, since its time-averaged neutron flux is generally less than that from reactors, one has to effectively elongate the incident pulse to obtain high effectiveness. Such an idea was proposed by Alefeld [3]. The proposed spectrometer includes a novel multi monochromator crystal, named as MUSICAL, which consists of several monochromators situated with a separation l_{M}. Suppose that a pulse of the width τ_{p} incident on the set of monochromators. The outgoing pulses have different flight length depending on the positions of the reflecting monochromators, and consequently become a set of pulses with a time separation of $\Delta t = 2l_\mathrm{M}/v_\mathrm{M}$, and with total duration of $n_\mathrm{M}\Delta t$. Each monochromator crystal has a slightly different lattice constant, so that each outgoing pulse has a slightly different energy. The outgoing pulses can be easily distinguished by arrival time at detectors if $\Delta t > \tau_\mathrm{p}$. Along this way, the short incident pulse is elongated effectively, with simultaneous incident-energy scan for a certain energy range determined by the number of the monochromators.

When applying this idea to the ultra-high energy resolution spectrometer using GaAs(200) reflections, however, one may encounter several problems. First problem may be the beam divergence. Provided that a practical goal of the total energy resolution of the spectrometer is $\Delta E \sim 0.03$ μeV, and thus $\Delta E \sim 0.021$ μeV for monochromator and analyzer separately. (Gaussian resolution functions are assumed for simplicity.) Then, the acceptable tolerance from exact backscattering at each device is about $\Delta\alpha \sim 0.26°$. This is less than the critical angle of Ni-coated guide tube ($\theta \sim 0.6°$ for $\lambda \sim 6$Å). Thus, the neutron beam from the guide tube cannot be used directly as incident neutrons, and instead, we have to focus the neutrons to obtain less beam divergence as suggested by Alefeld *et al.* [1]. Second problem may be the limited energy window. Assume a pulse repetition time as $T_\mathrm{p} = 40$ ms and a pulse width $\tau_\mathrm{p} \sim 250$ μs (JSNS coupled H_2 moderator). Then, the optimum length of the monochromator set (L_4) and consequently the radius of the secondary spectrometer (L_2) become $L_4 = L_2 = T_\mathrm{p}v_\mathrm{n}/4 \sim 7$ m for the neutron velocity $v_\mathrm{n} = 700$ m/s. Then the maximum number of monochromators is $n_\mathrm{M} = L_4/l_\mathrm{M} \sim 80$, which gives rise to the energy window of $0 < E < 2.4$ μeV. This is apparently too small. Third additional problem is considerable absorption of GaAs crystal, which simply prohibits us to use a large number of monochromator crystals.

In this study, we propose a combination of the multi monochromator crystal and Doppler drive as a possible solution for the ultra-high energy resolution backscattering spectrometer using GaAs(200). The geometrical restrictions to satisfy the above beam divergence requirement was estimated and shown to be feasible. The rough estimation on the neutron flux at sample position suggests that the present spectrometer give considerable neutron flux even with $\Delta E \sim 0.03$ μeV. The similar spectrometer with the Si(111) reflections is also studied and its efficiency is found to be 50 times better than the state-of-art spectrometer IN16.

2. Geometrical parameters

Figure 1 shows the schematic drawing of the proposed spectrometer, named as the Doppler-Musical spectrometer (D-M). Geometrical parameters are listed in Table 1. The spectrometer is mostly a superposition of the reactor-based backscattering spectrometer, such as IN16 [4], and MUSICAL [3]. Thus, principle features may be referred to the original articles, and here, we describe several modifications to realize the higher energy-resolution and efficiency.

As noted above, one must have an incident beam focused on the deflector and spherical monochromator centered at the focused point, to achieve a required exact backscattering condition ($\Delta\alpha \sim 0.26°$). The focused area should be as small as 13 mm × 13 mm. This focusing may be realized using a spherical supermirror focusing guide proposed by Mildner [5], however considerable effort may be required to minimize loss of neutrons at this device. The size of the monochromator is determined as 200 mm × 200 mm at $L_3 = 3$ m from the beam divergence after the deflector (reasonably 4° in view of critical angle of supermirror at 6Å). Each piece of the monochromator crystal should be less than 2 mm × 2 mm not to give considerable additional misalignment; such a spherical monochromator is produced recently for X-ray experiments [6].

The monochromatized neutrons from spherical monochromators are again focused into a small area and incident on the sample that is closely situated to the deflector. The sample size is, thus, limited by the beam size to about 13 mm × 13 mm. The radius L_2 may be restricted by rather practical requirements, such as size of neighboring instruments, and an acceptable maximum may be $L_2 \sim 4$ m. For this L_2, each piece of analyzer crystal can have a size of 5 mm × 5 mm. The counters should also have the same dimensions with the sample, and thus can be an array of half-inch ^{3}He detectors.

It is noteworthy that this spectrometer can select L_1 rather arbitrary. This flexibility is an outstanding feature when compared to the high-resolution time-of-flight spectrometers.

As checked above, the geometrical parameters are most likely in acceptable range, although several developments, in particular on the focusing guide, may be necessary.

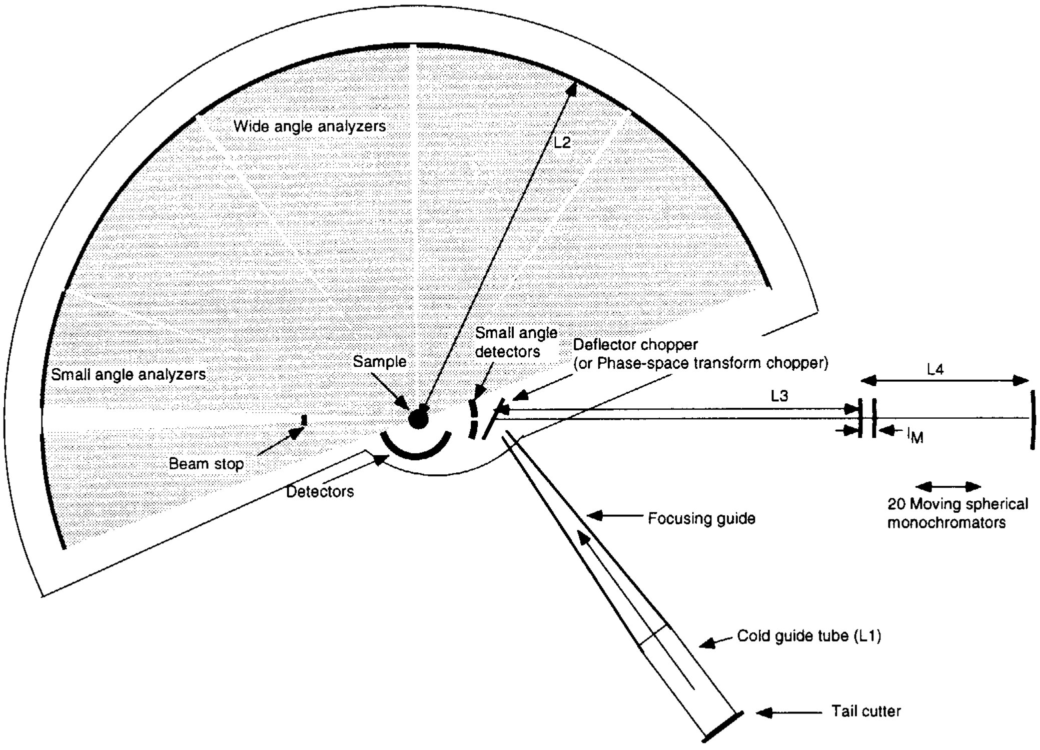

Figure 1: Schematic drawing of the Doppler-Musical spectrometer.

3. Multi monochromator crystal with a Doppler drive

To overcome the problems listed in the Introduction, the multi monochromator crystal is combined with the Doppler drive as shown in Fig. 2. The parameters are also listed in Table 1, which are determined as follows.

Since the extinction length of GaAs(200) is relatively large ($\Delta_h \sim 0.15\pi$ mm for $\lambda \simeq 5.65$ Å), the minimum thickness of each GaAs monochromator crystal may be about $d \sim 0.2$ mm [7]. Then, the reasonable number of the monochromators may be $n_{\rm M} \sim 20$, which gives a transmis-

Table 1: List of parameters for GaAs(200)

Parameter	estimated value
L_1	60 m (almost arbitrary)
L_2	4 m
L_3	3 m
L_4	2 m
Number of monochromators (n_{M})	20
Monochromator separation (l_{M})	100 mm
Focused area on deflector	13 mm × 13 mm
First monochromator size	200 mm × 200 mm
Last monochromator size	350 mm × 350 mm
Monochromator piece	2 mm × 2 mm
Sample size	13 mm × 13 mm
Analyzer piece	5 mm × 5 mm
Detector size	1/2 inch
Doppler frequency (f_{D})	$\sim$ 25 Hz
Doppler amplitude (a_{D})	$\sim$ 60 mm
Thickness of monochromator crystal	0.2 mm

sion factor of 0.7 for neutrons reflected at the last monochromator. Absorption by the holder of the monochromator crystals may not be negligible, but can be minimized by using Be. The total energy range covered by the n_{M} monochromators is $0.03 \times 20 = 0.6$ μeV. This range can be easily attained by temperature difference; the temperature difference between the first and last monochromators is roughly $\Delta T = 200$ K.

To enlarge the energy window to $-30 < E < 30$ μeV, one may use a Doppler drive with the frequency $f_{\mathrm{D}} \sim 25$ Hz and amplitude $a_{\mathrm{D}} \sim 6$ cm. We note that the drive can be synchronized to the pulse frequency so that the energy window can be fixed to a specified energy regions by tuning the phase of the drive. This may be a powerful technique if the energy region of interest is already known, such as for the measurements on the temperature dependence of tunnel peak or on the quasielastic peak width.

The apparent engineering problem is the Doppler drive for such a huge monochromator set. This may require a considerable effort on development of the driving mechanism. Other technical difficulty may be the temperature homogeneity of a monochromator.

4. Moderate energy resolution using Si(111)

If the energy-resolution requirement is relaxed to 0.3 μeV, one can use the Si(111) reflections in the present spectrometer. Parameters, determined along the same line as above, are listed in Table 3. The parameters are quite reasonable in contrast to the GaAs case. It should be noted that for the Si(111) case the focusing at the PG deflector, namely beam divergence at the deflector, is not so large. Thus, there is a possibility for further intensity gain by a novel phase-space transform chopper (PSTC) [8]. This device increases neutron density in energy space by using a moving PG deflector with the speed of about 300 m/s. The intensity gain can be a factor of about 4 [9]. Since we do not have serious geometrical restriction arising from the exact backscattering condition for this energy resolution, L_2 can be smaller than the GaAs case. Thus we choose $L_2 = 2$ m as a reasonable size, although longer L_2 (and accordingly L_4) can increase a duty cycle of this spectrometer.

Table 2: List of parameters for Si(111)

Parameter	estimated value
L_1	50 m (almost arbitrary)
L_2	2 m
L_3	2 m
L_4	2 m
Number of monochromators (n_{M})	25
Monochromator separation (l_{M})	100 mm
Focused area on deflector	32 mm × 32 mm
First monochromator size	140 mm × 140 mm
Last monochromator size	280 mm × 280 mm
Monochromator piece	2 mm × 2 mm
Sample size	32 mm × 32 mm
Analyzer piece	12 mm × 12 mm
Detector size	1/2 inch
Doppler frequency (f_{D})	$\sim$ 25 Hz
Doppler amplitude (a_{D})	$\sim$ 60 mm
Thickness of monochromator crystal	0.5 mm

5. Efficiency comparison

Table 3 shows rough estimates of gain/loss factors at each device compared to corresponding devices at IN16. The cold neutron source for the present spectrometer is assumed to be JSNS cold guide tube whose time-averaged neutron flux may be 1/4 of that at ILL. It can be seen that despite the difference in flux, the Doppler-Musical shows higher neutron flux at the sample position even with the GaAs(200) reflections. We should note that for this configuration the sample size is quite small as compared to that at IN16. Thus, if we take account of the sample size factor (3 cm × 4 cm for IN16 whereas 1.3 cm × 1.3 cm for D-M), the total neutrons at sample position is about 1/3 of IN16. This originates from the serious loss of neutrons at focusing guide assumed in the estimation; ideal focusing guide (i.e., its gain can be determined only by the geometry) gives focusing gain of about 60, which results in the six times higher total neutron intensity. Thus the development of the efficient neutron focusing technique is essential for the ultra-high energy resolution spectrometry. On the other hand, the spectrometer with the Si(111) reflections seems quite efficient compared to IN16; in fact, factor of about 50 can be expected. Therefore, by using Doppler-driven multi-monochromator-crystal, one may obtain efficient spectrometer with reasonable geometrical dimensions.

5. Conclusion

Table 3: Comparison of gain/loss factors at each device

Device	D-M(GaAs)	D-M(Si)	IN16 (polished Si)
Source	0.25	0.25	1
First deflector	1.3 (no deflector)	1.3 (no deflector)	1
Focusing guide	2 (gain 10)	1 (gain 5)	1 (gain 5)
Second deflector	1	4 (PSTC)	1
Monochromator (n_M)	20	25	1
Monochromator (ΔE)	0.1 ($\Delta E \sim 0.03\ \mu$eV)	1 ($\Delta E \sim 0.3\ \mu$eV)	1 ($\Delta E \sim 0.3\ \mu$eV)
Duty cycle	2	2	1
Total	2.1	52	1

We have suggested that the combination of multi monochromator crystal and Doppler drive, together with the focusing techniques, can realize the backscattering spectrometer with ultra-high energy resolution of $\Delta E \sim 0.03\ \mu$eV using the GaAs(200) reflections and with the reasonable energy range $-30 < E < 30\ \mu$eV. On the other hand, a moderate energy resolution ($\Delta E \sim 0.3\ \mu$eV) spectrometer using the Si(111) reflections can be obtained with reasonable dimensions. Although a number of engineering issues must be overcome, intensity estimations suggest that the Doppler-Musical spectrometer can be a possible choice for the high-energy resolution spectrometer at the spallation neutron source.

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References

[1] B. Alefeld, T. Springer, and A. Heidemann, Nucl. Sci. and Eng. **110** (1992) 84.

[2] B. Alefeld, L. Dohmen, and A. Heidemann, Physica B **283** (2000) 299.

[3] B. Alefeld, Nucl. Instr. and Meth. A **355** (1995) 478.

[4] B. Frick, A. Magerl, Y. Blanc, and R. Rebesco, Physica B **234-236** (1997) 1177.

[5] D. F. R. Mildner, Nucl. Instr. and Meth. A **297** (1990) 38.

[6] B. Frick, private communication.

[7] V. F. Sears, *Neutron Optics* (Oxford University Press, New York, 1989).

[8] J. Schelten, and B. Alefeld, Julich Report 1954 (1984) p. 378.

[9] Detailed descriptions on the phase-space transform chopper can be found at the web site: http://www.ncnr.nist.gov/instruments/hfbs/