Journal of Neutron Research, March–September 2005 Vol. 13 (1–3), pp. 189–192

High-energy-resolution Option for the Inverted-geometry Time-of-flight Spectrometer DYANA

TAKU J. SATO[a,*] and KAORU SHIBATA[b]

[a]*National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan;* [b]*Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195, Japan*

DYANA is an inverted-geometry time-of-flight (TOF) spectrometer proposed for the Japan Proton Accelerator Research Complex (J-PARC) project. Here, we show that by introducing pulse-shaping disk choppers and Si 111 analyzer, a DYANA-type short-incident-flight-path spectrometer can attain a very high energy resolution of 2 μeV, with an acceptable neutron flux at the sample position.

Keywords: Inverted-geometry spectrometer; High-energy resolution; Backscattering; J-PARC

INTRODUCTION

DYANA is an inverted-geometry time-of-flight (TOF) spectrometer proposed for the Japan Proton Accelerator Research Complex (J-PARC) project [1,2]. The primary purpose of DYANA is to study dynamical aspects of biomolecules and proteins in wide energy and momentum-transfer (Q) ranges, which may hopefully reveal fundamental relations between microscopic atomic motions of these complex systems and their functions. Due to limited volumes of specimens, an inelastic scattering spectrometer with an extremely-high counting rate is desired. Thus, DYANA is designed so as to maximize the counting rate at the reasonable cost of energy and Q resolutions; high reflectivity of nearly backscattering (NBS) PG 002 analyzers and the short incident flight path ($L_1 = 32\,\mathrm{m}$) provide possibly the highest counting rate among several types of low-energy inelastic scattering spectrometers proposed for the J-PARC project. The energy resolution is moderate, being 15 μeV at the elastic position, which is, however, not so miserable when considering its wide energy (dynamic) range of up to $\sim 14\,\mathrm{meV}$.

On the other hand, there is a continuous necessity for a higher energy resolution, such as $\Delta E \sim 2\,\mu\mathrm{eV}$, mainly for elastic incoherent scattering factor measurements. At spallation neutron sources, such a high-energy resolution may conventionally be achieved by using perfect crystal Si 111 reflections as an analyzer in NBS geometry, combined with the short pulse shape of decoupled and poisoned moderator and with a long primary flight path [3].

*Corresponding author. Present address: Neutron Science Laboratory, Institute for Solid State Physics, University of Tokyo, 106-1 Shirakata, Tokai, Ibaraki 319-1106, Japan. Tel.: +81-29-287-8905. Fax: +81-29-283-3922. E-mail: taku@issp.u-tokyo.ac.jp

ISSN 1023-8166 print/ISSN 1477-2655 online
DOI: 10.1080/10238160412331299924

(We refer to this type of spectrometer as the Long-L_1 spectrometer.) In this study, we will show that this 2 μeV resolution can be also realized with acceptable neutron flux, by introducing the pulse-shaping disk choppers [4] and Si 111 analyzer to the DYANA-type Short-L_1 spectrometer. Since the spectrometer thus obtained is compact in size, covers a very wide dynamic range from 2 μeV to 14 meV, and requires only minor modifications from the original DYANA design, this may be a cost-effective way to realize 2 μeV neutron spectroscopy, compared to building a separate spectrometer dedicated to high-energy-resolution experiments.

EFFICIENCY ESTIMATION: MONTE CARLO (MC) SIMULATION DETAILS

Secondary spectrometer configurations for the Long-L_1 and Short-L_1 spectrometers are, in principle, identical; the Si 111 reflections are used as analyzer in NBS geometry, with detectors placed in vicinity of the sample. Owing to this identity, we may directly compare efficiencies of the two different spectrometers by simply comparing their sample position neutron fluxes. The fluxes were estimated using the Monte Carlo (MC) ray-tracing code `McStas` [5]. The primary spectrometers are depicted in Fig. 1, whereas their parameters are given in Table I. We assumed decoupled-and-20 mm-poisoned (port 9) and decoupled (port 11) moderators of the J-PARC neutron source running at 1 MW for the Long-L_1 and Short-L_1 simulations, respectively; the two different moderators were assumed in order to directly compare estimated sample-position-neutron fluxes of the two different type spectrometers. Several supermirror guide tubes, including a converging guide funnel in front of the sample, are placed in the incident beam line, as are expected to be done for the DYANA spectrometer. The supermirrors are assumed to have $3Q_c$ reflectivity. For the Long-L_1 spectrometer, the incident

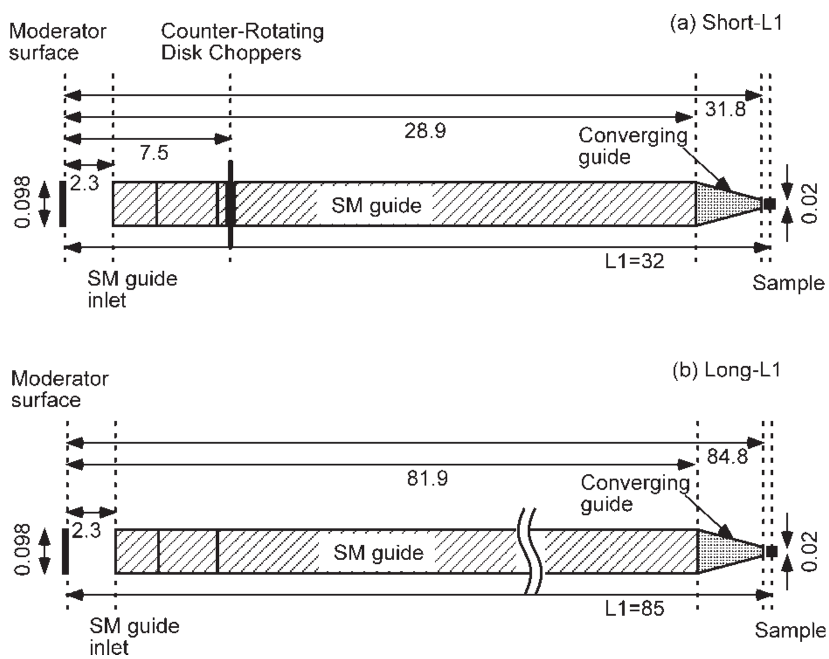

FIGURE 1 Schematic illustrations of primary spectrometers: (a) the Short-L_1 spectrometer; (b) the Long-L_1 spectrometer. (Lengths are in meter units.) The primary spectrometers are symmetric for horizontal and vertical directions perpendicular to the neutron beam line, except for an asymmetry of the chopper windows in (a), which has a dimension of 0.1 m in height and 0.02 m in width.

TABLE I Parameters of the Long-L_1 and Short-L_1 spectrometers

	Long-L_1	*Short-L_1 (DYANA 2 μeV)*
Moderator	Decoupled-poisoned	Decoupled
L_1 (m)	85.0	32.0
Guide cross section (m^2)	0.098 × 0.098	0.098 × 0.098
Converging guide length (m)	2.9	2.9
Supermirror	$3Q_c$	$3Q_c$
Counter-rotating-disk-chopper position (m)	N/A	7.5
Counter-rotating-disk-chopper frequency (Hz)	N/A	300
Counter-rotating-disk-chopper-window width (m)	N/A	0.02
Counter-rotating-disk-chopper radius (m)	N/A	0.3
Inner width of guide tube at chopper (m)	N/A	0.098
Source pulse width at 2 meV (μs)	39	83
Chopped pulse width at 2 meV (μs)	N/A	18
Guide end to sample (m)	0.2	0.2
Sample size (m^2)	0.02 × 0.02	0.02 × 0.02

beam line comprises only the supermirror guide sections, whereas the Short-L_1 spectrometer has an additional counter-rotating pair of two disk choppers at $L = 7.5$ m, which shape relatively wide pulses of the decoupled moderator into the desired width of about 18 μs. To realize this pulse width, a narrow chopper windows of 0.02 m are necessary due to limitations of present chopper technology; counter-rotating disk choppers with a radius $R = 0.3$ m operating at 300 Hz are the best we can expect at the present moment. The narrow window and short opening time give rise to apparent neutron loss, nevertheless, our simulation in the following suggests that this loss would be largely compensated by higher flux of the non-poisoned moderator, as well as high transportation efficiency of the shorter guide tube.

In the MC simulations, we generate 10^6 (Long-L_1) or 10^7 (Short-L_1) incident neutrons in an energy range of $1.999 < E < 2.001$ meV (2 μeV range). The TOF spectra are recorded at the sample position, and then the spectra are converted to energy spectra, using the following equation:

$$E = \frac{1}{2} m_N \left(\frac{L_1}{t_s}\right)^2 \simeq (5.227 \times 10^{-6}) \left(\frac{L_1}{t_s}\right)^2 \text{ (meV)} \tag{1}$$

where m_N and t_s are the neutron mass and TOF at the sample position, respectively. It is noteworthy that the neutron generation in the 2 μeV range approximately corresponds to placing an analyzer with a 1 μeV resolution, which roughly equals to the NBS Si 111 resolution. Therefore, a peak width in the energy spectrum may provide an estimate of the total energy resolution, including both the finite incident-pulse-width effect and the finite analyzer resolution.

RESULTS AND DISCUSSION

The sample-position energy spectra for both the spectrometers are shown in Fig. 2. The energy resolution of the Short-L_1 spectrometer becomes 1.82(2) μeV when the disk choppers run at 300 Hz, which is comparable to the resolution [2.04(7) μeV] of the Long-L_1 spectrometer. Therefore, the 2 μeV resolution is achievable using existing disk chopper technology. In addition, owing to the higher flux of the decoupled (non-poisoned) moderator, regardless of the narrow opening of the disk choppers, the sample position flux of the Short-L_1 spectrometer is acceptable, being 1/3 of the Long-L_1 spectrometer. This confirms that the disk choppers and Si 111 analyzer are feasible options for the DYANA spectrometer to

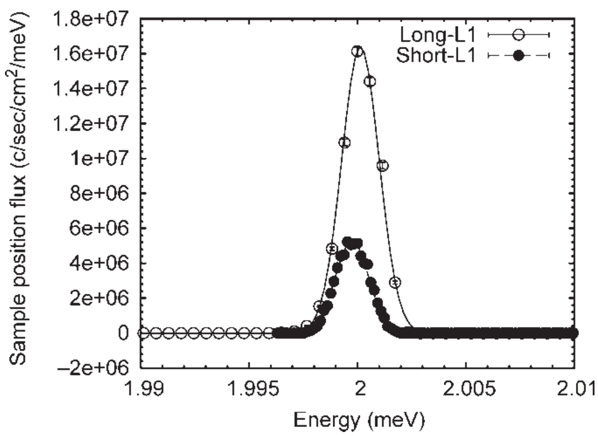

FIGURE 2 Sample position neutron flux comparison between the Long-L_1 and Short-L_1 spectrometers.

enable 2 μeV spectroscopy. One drawback may be a limited energy scan range; the 300 Hz disk choppers at $L = 7.5$ m limit the scan range to $-20 < E < 20$ μeV. However, since the normal PG 002 mode of DYANA provides considerably wide energy range of up to ~14 meV, complementary use of the PG 002 and 2 μeV modes can overcome this energy window limitation.

In the present study, we have shown that the 2 μeV resolution can be realized by slightly modifying the DYANA spectrometer; only pulse-shaping disk choppers and an Si 111 analyzer are to be introduced. The sample position flux estimation shows that the 2 μeV mode of the DYANA-type Short-L_1 spectrometer gives roughly 1/3 flux of the Long-L_1 spectrometer, assuming J-PARC moderators and identical secondary spectrometers. It should be noted that we design the 2 μeV option so as not to spoil the original DYANA concept, i.e. the higher counting rate with the moderate energy resolution. Consequently, the 2 μeV mode, we proposed here, is not perfectly optimized; DYANA is, in its basic concept, primarily optimized for the 15 μeV mode. Nevertheless, our simulation indicates that the disk choppers and Si 111 analyzers will be useful options, providing an opportunity to perform 2 μeV resolution experiments using DYANA with reasonable neutron flux.

REFERENCES

[1] Shibata, K. *et al.* (2003) "High efficiency indirect geometry spectrometer: DYANA dedicated for biomolecular dynamics at JSNS". *Presented at the International Symposium on Pulsed Neutron Science and Instruments* (IPN2003) (Tsukuba, Japan, 2003).

[2] Shibata, K., Tamura, I., Soyama, K., Arai, M., Middendorf, D. and Niimura, N. (2003) "High efficiency indirect geometry crystal analyzer TOF spectrometer: DYANA dedicated to biology, planning in JSNS", in *Proceedings of the 16th Meeting of the International Collaboration on Advanced Neutron Sources*, Code I33.

[3] Bordallo, H.N., Herwig, K.W. and Zsigmond, G. (2002) "Analytical calculations and Monte-Carlo simulations of a high-resolution backscattering spectrometer for the long wavelength target station at the spallation neutron source", *Nucl. Instrum. Methods A* **491**, 216.

[4] Russina, M., Mezei, F. and Trouw, F.R. (2001) "New capabilities in spectroscopy on pulsed sources: adjustable pulse repetition rate, resolution and line shape", in *Proceedings of the Fifteenth Meeting of the International Collaboration on Advanced Neutron Sources*, JAERI-Conf. 2001-002, p. 349.

[5] Lefmann, K. and Nielsen, K. (1999) "A general software package for neutron ray-tracing simulations", *Neutron News* **10/3**, 20, also see the McStas WWW home page: http://neutron.risoe.dk/mcstas/.