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Status report of the chopper spectrometer 4SEASONS

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Abstract. 4SEASONS is a medium-resolution thermal neutron chopper spectrometer in the Materials and Life Science Experimental Facility (MLF) at J-PARC. Although 4SEASONS is routinely used for many experiments by internal and external users, upgrading and maintenance work is still underway. This paper reviews the recent improvements of the instrument.

1. Introduction

4SEASONS (or *SIKI*) is a time-of-flight direct geometry chopper spectrometer in the Materials and Life Science Experimental Facility (MLF) at the Japan Proton Accelerator Research Complex (J-PARC) [1]. It is installed at BL01 beam port viewing the coupled moderator which is 18 m upstream from the sample position. The incident neutrons are monochromatized by a fast-rotating Fermi chopper positioned at 1.7 m upstream from the sample position. In addition, the instrument has a T0 chopper for suppressing fast neutrons and two disk choppers for band definition. Neutrons scattered by samples are detected by the ^{3}He position sensitive detectors placed at 2.5 m from the sample position. 4SEASONS is designed for measurements of spin and lattice dynamics in the 10^0–10^2 meV energy range. The instrument has been used by researchers from a variety of countries for studies of magnetic and lattice dynamics in condensed matters such as superconductors, magnetic materials, dielectrics, catalysts, and thermoelectric materials. Upgrading and maintenance work is still ongoing, which will improve the performance, usability, and safety of the instrument. In this paper, we review the improvements of the instrument achieved in the recent two years for the Fermi chopper, detector system, sample environments, and software.

2. Newly developed Fermi choppers

The original Fermi chopper of 4SEASONS holds a slit package with 65 mm × 70 mm cross-section and 100 mm depth. Its designed maximum rotation frequency was 600 Hz [1]. However, in 2011, the rotation was found to be unstable at high frequencies because of a secular change in the slit package, and we limited the rotation frequency at 350 Hz and lower. This situation severely restricted the available energy resolution, especially for high-energy experiments. Accordingly, we developed a new Fermi chopper, which was manufactured by MIRROTRON Ltd. and SKF Magnetic Bearings. The new Fermi chopper has a more compact slit package with cross-section and depth of 58 mm × 53.4 mm and 20 mm, respectively. The spacing of the slits is designed so that it gives the same energy resolution as the original chopper. The new chopper can rotate stable up to 600 Hz because of its compact design. Figure 1(a) shows the energy spectra of $C_4H_2I_2S$ at 5 K measured with the incident energy E_i = 220 meV and the

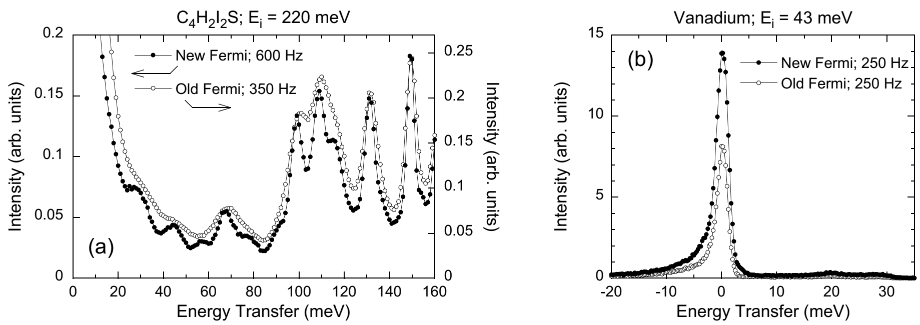


Figure 1. Comparison of energy spectra measured with the old and new Fermi choppers. (a) Energy spectra of $C_4H_2I_2S$ at 5 K measured with $E_i = 220$ meV. Scattering intensities were integrated over $Q = 6$–11 Å^{-1}. Solid and closed circles show data measured with the new Fermi chopper rotating at $f = 600$ Hz and old chopper rotating at $f = 350$ Hz, respectively. (b) Energy spectra of vanadium measured with $E_i = 43$ meV and $f = 250$ Hz. Scattering intensities were integrated over $Q = 3.4$–5.0 Å^{-1}. Solid and closed circles show data measured with the new and old Fermi choppers, respectively.

maximum achievable rotating speeds for both the choppers, i.e., $f = 350$ Hz and 600 Hz for the old and new choppers, respectively. The high-speed rotation of the new Fermi chopper considerably improves the data quality. It provides better peak separations and improved signal-to-noise ratio in the low-energy region, where inelastic scattering intensity often suffers from the tail of elastic scattering.

Another important benefit of the shallow depth slits is that the chopper provides much higher neutron transmission than the original chopper. Figure 1(b) shows a comparison of the energy spectrum of vanadium measured with the new and old Fermi choppers. In this example, the choppers rotate at $f = 250$ Hz to produce the incident energy $E_i = 43$ meV. The new Fermi chopper gives 1.7 times higher peak intensity than the old chopper, whereas the peak width is almost identical for both the choppers. The intensity gain by the new chopper becomes particularly high for low energy neutrons and high rotation speeds. (For example, it reaches 17 for 18 meV and 300 Hz.) This feature expands the practical energy range for the multi-E_i measurements [2]. Notably, Fig. 1(a) also proves the high transmission of the new chopper. The data for the new chopper have a comparable intensity with that for the old chopper in spite of the much higher speed of rotation in the former.

In parallel, we are developing another Fermi chopper, called MAGIC chopper, which utilizes supermirror-coated slits [3–5]. In late 2014, we tested the prototype of the MAGIC chopper on BL01. Unfortunately, we found that the obtained neutron flux was much lower than the expected value. Nevertheless, we could verify the basic performance of this type of chopper. We performed Monte Carlo simulations to find that the low neutron flux is mainly caused by the low reflectivity of the supermirrors. We are currently developing a new slit package with higher-reflectivity supermirrors.

3. Detectors

Partial recovery of the detector deficiency. The detector banks of 4SEASONS cover a scattering angle in the range of −35.3° to +130.5° in the horizontal plane [1]. However, the detector banks are not fully occupied due to the recent shortage and resulting high price of ^{3}He gas. The initial number of detectors was 191 pieces covering the range of −35.3° to +54.5° in the horizontal plane. In 2013–2015, we installed 75 pieces of detectors [Fig. 2(a)]. The maximum horizontal scattering angle is currently +90.7°. The newly installed detectors expanded the accessible momentum transfer (Q) as shown in Fig. 2(b). This value is still lower than the designed one, and a further increase in detectors is undoubtedly important. However, for studies on low-dimensional systems in which only some particular crystal axes are of interest, these axes are often set perpendicular to the incident beam. In such a case, the scattering angle of 90° can provide the maximum Q range.

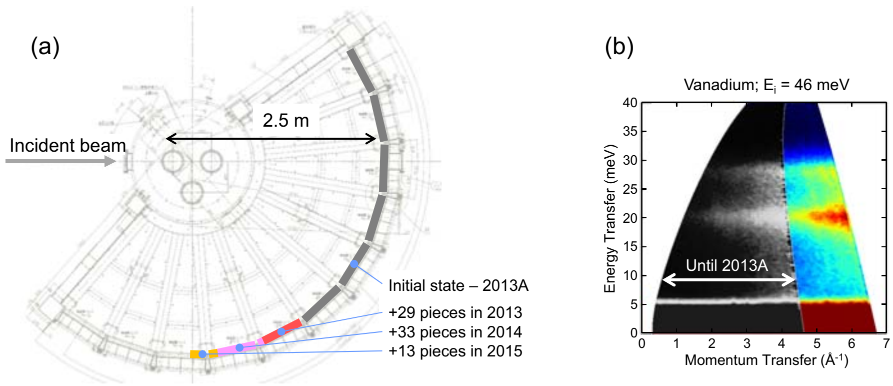


Figure 2. (a) Top view of the vacuum scattering chamber of 4SEASONS and the detector banks where detectors are installed. Detector banks indicated by gray thick lines show the initial detector arrangement. Detector banks colored in red, pink, and orange show the positions where detectors were installed in 2013, 2014, and 2015, respectively. (b) Momentum (Q)-energy (E) map of inelastic scattering spectra of vanadium measured with $E_i = 46$ meV. The areas displayed with a gray scale and with a color scale show the Q-E regions covered by the initially installed detectors and newly installed detectors, respectively.

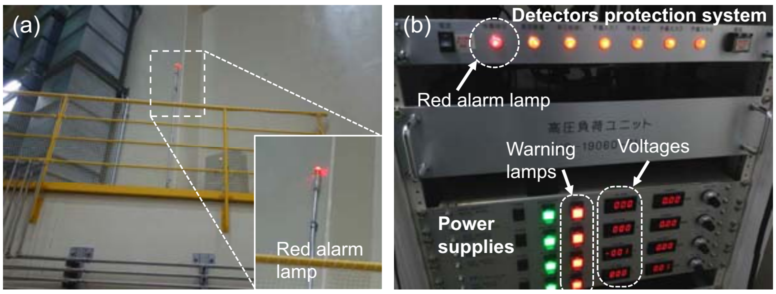
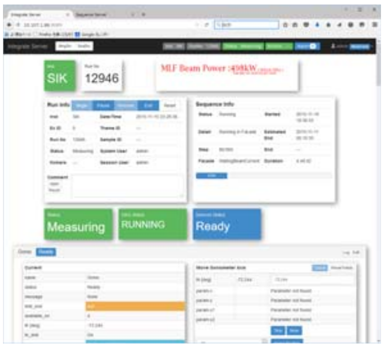


Figure 3. (a) Seismometer in MLF. (inset) The red alarm lamp is on by detecting an earthquake. (b) The detector protection system and the new high-voltage power supplies for detectors in the 4SEASONS cabin.

Detector protection. ^{3}He detector is vulnerable to vibration, especially when the electric power is supplied. Our experience with the big earthquake in 11 March 2011 reminded us of the importance of the protection of the detectors against earthquakes. Accordingly, in 2015, we introduced an interlock system to prevent detector damage caused by that type of disaster. This system is connected to seismometers placed in the experimental halls. Once it detects an earthquake whose intensity is bigger than some specified value (currently bigger than 4 on the Japanese seismic scale), it cuts the electric power supply to the detectors. The interlock system is expandable to adopt other input signals of incidents such as an unexpected vacuum break. In addition, we replaced the power supplies for the detectors with new ones which are more compatible with the interlock system. The new power supplies can cut off the power within 5 seconds. The practical shutdown time is longer depending on the capacitance of the detector electronics, and we have never experienced any damage on the detectors by the shutdown. Figure 3(a) shows the seismometer in the No. 1 Experimental Hall of MLF, which lit up its red warning lamp by detecting an earthquake with a seismic intensity of 4 on 22 November 2016. It successfully cut off the power supply to the detectors as shown in Fig. 3(b).

4. Sample environments

Preparing for magnet. To date, no magnets are available on 4SEASONS. However, the dimension of the sample environment attachment flange of the scattering chamber can accommodate the commonly-used 7-T magnet in MLF. One of the difficulties in operating magnets is that many iron components surround the sample area. Moreover, the turbomolecular pumps with magnetic bearings are attached just below the sample position, and we must be careful of the influence of the stray field on these pumps.

(a)


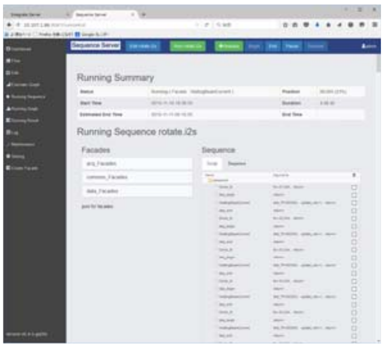
(b)


Figure 4. Web interfaces of the new instrument control system of 4SEASONS. (a) Integrate Server to control the devices and run measurements. (b) Sequence Server to manage measurement sequences.

Thus, we investigated stray fields using the computer aided engineering system Femtet®, considered the iron components, and evaluated the field intensity on the turbomolecular pumps. To validate our calculations, we operated the commonly-used magnet on 4SEASONS for the first time, and measured the intensity of the magnetic field at several points around the magnet. Although the maximum applied field in this test operation was only 1 T, the observed values were consistent with the calculations. Numerical calculations of the stray field are currently underway to find an appropriate measure to protect the turbomolecular pumps against the field and estimate the maximum available field on the instrument.

Improvement in the oscillating radial collimator. To reduce background scattering from the sample environment, 4SEASONS can be equipped with an oscillating radial collimator (ORC), which was developed by the Technology Development Section of MLF. It has a number of thin shielding blades made of cadmium-plated aluminum sheets, which surround the space for the sample environment device. The ORC is installed on the vacuum scattering chamber, and it is usually oscillated horizontally to avoid uneven intensity distribution on the detectors caused by shadows from the shielding blades [6]. However, this type of oscillation is not simple, because the unevenness in intensity depends on the oscillating speed and angle. Even after optimizing these parameters, we found that the shielding blades inevitably made shadows when they stopped at both ends of oscillating angle to change the oscillating direction, even though the dead time was small (~20 ms). To solve this problem, we recently developed a new oscillating mode, called "shift-mode", which can shift the oscillating angle range gradually. We confirmed that by changing the angle range by 0.1° per oscillation, we can obtain more even intensity distribution than the normal oscillating mode.

5. Softwares

New instrument control system. Many of the instruments in MLF, including 4SEASONS, utilize instrument control systems based on the control software framework IROHA [7]. A new control software framework, called IROHA2, was recently developed by the MLF Computing Environment Group to replace IROHA [8]. We developed a new instrument control system based on IROHA2, which has been available for user experiments since autumn in 2015. This control system has a web-based user interface, which allows users to control the instrument intuitively and remotely from any place connected to the server through LANs (Fig. 4). Registered users (currently they are limited to instrument group members) can view the instrument status even from their smart phones. The user interface is not the only benefit of the new control system. Another important feature of the new control system is that it enables us to control different devices uniformly and introduce new devices easily. This feature is particularly useful when a nonstandard sample environment is used on the instrument.

4D mapping by continuous rotation of single crystal samples. One of the recent trends in experiments on a single crystal using a chopper spectrometer is to grasp whole excitations in the 4D energy-momentum space by rotating the crystal over a wide angular range. The data analysis software suite

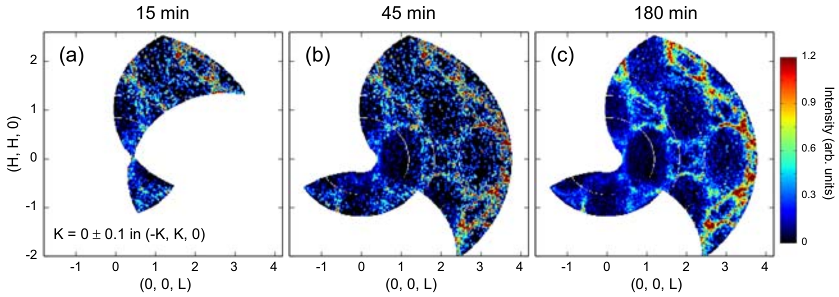


Figure 5. Phonon spectra of a single crystalline copper obtained by continuously rotating the crystal. The crystal was rotated horizontally at a rate of 160°/h. (a), (b), and (c) show the constant E slices at $E = 13 \pm 1$ meV, 15, 45, and 180 min after the start of the measurement, respectively.

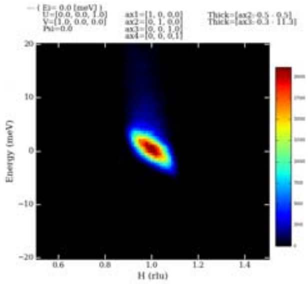


Figure 6. Example of the resolution function for 4SEASONS, simulated and displayed using McStas and Utsusemi, respectively.

in MLF, Utsusemi, is compatible for such measurements [9], which makes 4D mapping a routine at 4SEASONS. So far, implementation in Utsusemi has not been so flexible, because a crystal has been rotated stepwise with a small (0.5°–1°) step angle. For such a step-by-step rotation, the angular range and step size of the rotation have to be determined before the measurement. Real-time visualization of acquired data, which is often important to decide whether the current measurement is successful, is difficult. On the other hand, the data acquisition system of MLF based on event data recording can potentially provide flexibility in crystal-rotating measurements. The 4D mapping by continuous rotation of a single crystal was recently developed at the ARCS spectrometer at the Spallation Neutron Source utilizing the event data recording [10]. Recently, a new measurement and analysis system for crystal-rotating measurements, which maximizes the potential of the event data recording, was developed by the MLF Computing Environment Group. This system takes advantage of the data acquisition electric module, TrigNET [11], and a data processing function called online monitor [12]. The former can record any sample environment information as events synchronized with neutrons, whereas the latter enables pseudo real-time data visualization by incremental data analysis. With these features, we can perform 4D mapping by continuously rotating a single crystal without determining the step size in advance and then visualize the data in real time. The new system has been incorporated in Utsusemi, and we introduced it on 4SEASONS in late 2016. Figure 5 shows the phonon spectra of a single crystal of copper measured by continuously rotating the crystal using the new system. Given the online monitor functionality, we can observe the progress of the measurement. By rotating the crystal at a reasonably fast speed, we can obtain the rough picture at an early measurement stage [Figs. 5(a) and 5(b)]. The statistics improves with time by repeating the rotation [Fig. 5(c)], and we can stop the measurement anytime soon after the statistics reaches the required level. These features are useful to optimize the measurement condition and determine the experiment plan.

Instrument resolution. Estimation of instrumental resolution is important for neutron scattering instruments to derive physical quantities from the experimental data. We have already established the estimations of 1D energy and momentum resolutions for 4SEASONS, i.e., energy resolution for incoherent scattering and momentum resolution for powder samples [13, 14]. In general, however, the resolution function for inelastic neutron scattering instruments is expressed as an ellipsoid in the 4D momentum and energy space. Recently, numerical methods to evaluate the resolution by Monte Carlo simulation have been developed [15–18]. This type of method can be easily applied to complicated instruments, and detail shape of the resolution function such as tail due to the moderator time structure can be reproduced. A novel method to estimate the resolution function of 4SEASONS using the Monte Carlo simulation package McStas [15, 16] is currently under development. Another important issue for resolution analysis is how to visualize the 4D resolution function. Traditionally, an ellipsoid defining the half values of the resolution functions is displayed as functions of momentum axes parallel and perpendicular to the scattering vector. However, this general way of representation is not always convenient to compare the resolution with experimental data. For this purpose, we modified the *Q*-*E* visualizer in Utsusemi [9] to accommodate it to the resolution data generated by the McStas simulation [19]. Subsequently, the simulated resolution functions can be displayed in the same manner as a single crystal experiment. Figure 6 shows an example of a simulated resolution function displayed on a 2D map, defined by energy transfer and one of the principal axes in the reciprocal lattice. An overall feature of the inclined ellipsoid is clearly captured. The widths of the simulated resolution functions show reasonable agreements with the values obtained by simple analytical calculations, thereby validating the performed Monte Carlo simulation [19]. Moreover, a tail of the resolution function extending toward high energies is also visualized. Although the integration of the McStas simulation and Utsusemi visualization is still primitive, we continue developments to improve the integration.

6. Summary
We reviewed recent improvements in the 4SEASONS spectrometer at MLF in J-PARC. The performance of the Fermi chopper and the coverage of the detectors remarkably improved. The sample environment and software were also developed in their performances and usability. Protecting the instrument against hazards is important, and we have made progress in this aspect by developing detector protection.

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