Current status of a time-of-flight single crystal neutron diffractometer SENJU at J-PARC

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Abstract. SENJU is a state-of-the-art single crystal time-of-flight Laue diffractometer in Materials and Life Science Experimental Facility at Japan Proton Accelerator Research Complex (J-PARC). The diffractometer is designed for precise crystal and magnetic structure analyses under multiple extreme conditions, such as low temperature, high-pressure, high-magnetic field. Measurements using small sample less than 1.0 mm³ will be also realized, which allows us to study wide variety of materials. SENJU is using a poisoned decoupled moderator to obtain peak profiles of Bragg reflection, and intensity distributions of superlattice reflections and diffuse scatterings with good accuracy. At the beginning, the diffractometer will have 31 two-dimensional scintillator detectors to cover wide area of reciprocal lattice space by a single measurement. The instrument is currently under construction and is scheduled to start on-beam commissioning in February 2012.

1. Introduction

Crystal structure is one of the most fundamental properties of materials and closely relates with physical characteristics. Detailed information on the structure and its external-field response are indispensable to understand and to control physical properties of the materials. Diffraction experiments are a basic but an essential method for the structural study of the materials.

Time-of-Flight (TOF) single crystal neutron diffraction gives us an efficient way to precisely analyse the crystal and magnetic structures and structural fluctuation of the materials. SXD at ISIS [1] has been a leading instrument in this field for decades, and TOPAZ at SNS [2] has been just launched. At Materials and Life Science Experimental Facility at Japan Proton Accelerator Research Complex (MLF/J-PARC), construction of a TOF single crystal neutron diffractometer SENJU has been started in 2010. The primary aim of SENJU is precise crystal and magnetic structure analyses under multiple extreme conditions. SENJU also sheds light on superlattice reflections and diffuse scatterings in order to analyse local structures as well as phase transitions of the materials. Measuring a small sample, less than 1.0 mm³, is another important feature of this diffractometer. SENJU will be able to extend a range of materials that can be measured by neutron diffraction method in the field such as science and engineering. In this paper, overview and current status of SENJU are presented.

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2. Instrument design

2.1. General design of diffractometer
Choice of the moderator is one of the most crucial decisions made in the first stage. To meet the targeted science at SENJU, a poisoned decoupled moderator was selected since it provides a symmetrical pulse shape and resultant better S/N ratio at the pulse tail compared with other types of moderators. The sample position is set to be 34.8 m from the moderator. As for the high-resolution capability, Δd/d < 0.2 % will be easily achieved by the high-angle detectors at this position. A bandwidth of 4.4 Å should be adequate for the most of the experiments at SENJU. A straight beamline was adopted instead of a curved one due to the necessity of short wavelength neutrons, up to 0.4 Å (500 meV). A uniform beam divergence of ± 0.30° at the sample position will be realized by an elliptical shape neutron guide, as briefly described in the next paragraph. The distance between the sample and the detector banks is set to be 0.8 m in minimum, which can be extended up to 1.3 m to incorporate various accessories and to realize better spatial resolution. An exchangeable vacuum sample chamber is employed to accept a superconducting magnet and to simplify a beam alignment process. Figure 1 shows the illustration of the chamber and detectors array of SENJU. General specifications of SENJU are listed in table 1.

Figure 1. 3D illustration of SENJU

| Table 1. General specifications of SENJU |
|----------------------------------------|
| Beamline | BL18 |
| Moderator | Decoupled poisoned H₂ (20 K) |
| Neutron wavelength | 0.4 ~ 4.4 Å (1st frame) |
| | 4.6 ~ 8.8 Å (2nd frame) |
| Sample position | 34.8 m from moderator |
| Guide tube | Straight elliptic supermirror |
| Detector | WLSF-type scintillator detector |
| | 4 × 4 mm² / pixel |
| | 0.8 m or 1.3 m from sample |
| Range of 2θ | -13° ~ -167°, +58° ~ +167° |
| Beam divergence | ± 0.30° (Standard mode) |
| | ± 0.45° (High-intensity mode) |

2.2. Beamline layout
The beamline of SENJU is designed to transport neutrons of $\lambda = 0.4$ Å at the minimum with a uniform divergence to the sample position. A square cross-sectional elliptic straight neutron guide is adopted where focal points of the guide are 9.8 and 34.8 m from the moderator. The start and the end positions of fixed section of the guide are 15.2 and 31.8 m, respectively. The optical components to control beam divergence and size consist of a subsequent interchangeable section of the guide (supermirror coating $m = 5$) and two $\text{B}_4\text{C}$ slits as shown in figure 2. The beam divergence will be increased from $\pm 0.30^\circ$ to $\pm 0.45^\circ$ by the use of this section with a little extension of the minimum wavelength. A better collimation, i.e., the divergence smaller than $\pm 0.30^\circ$, will be realized by use of the slits with a compensation of the neutron flux. Bandwidth choppers are necessary to select a single frame of 4.4 Å and eliminate other frames. Instead of the use of the second frame, a double frame mode with a half repetition will be effective in some experiments. So-called $T_0$ chopper is also necessary to stop fast neutrons and prompt $\gamma$-ray from the moderator for experiments using a sensitive sample. To optimize parameters of the beamline components, such as the guide, choppers and slits, Monte Carlo simulations were carried out using the program McStas [3]. Note that the simulated beam profile showed that the beam halo does not exceed $30 \times 30$ mm$^2$ at the sample position without the slits. A schematic drawing of the beamline layout of SENJU is shown in figure 2.

Figure 2. Schematic drawing of the beamline layout of SENJU

2.3. Detector system

The success of SENJU depends on the reliability and stability of the detector system. Recently, a scintillator detector has been an only choice for the diffractometer because of shortage of $^3\text{He}$ gas. A wavelength-shifting fiber (WLSF) -type scintillator detector developed by Japan Atomic Energy Agency [4] is already in operation at the biological TOF single crystal neutron diffractometer iBIX [5] in MLF/J-PARC. This type of detector satisfies the required performance for SENJU, such as spatial resolution and count capability. Due to the experimental requirements, the pixel size of the detector was relaxed for SENJU to $4 \times 4$ mm$^2$ from $0.52 \times 0.52$ mm$^2$ of the iBIX detector. A sensitive area of the detector was widened for SENJU to $256 \times 256$ mm$^2$ from $133 \times 133$ mm$^2$ of iBIX. A chassis size of the detector was also changed to $300 \times 300$ mm$^2$ from $160 \times 160$ mm$^2$. Reliability and stability of the system were improved and the relative dead area was reduced by these modifications. The Monte Carlo simulation using McStas showed that at least $3 \times 3$ pixels were illuminated for a Bragg spot from an ideal single crystal, and in reality $5 \times 5$ or more pixels will detect the spot. At the maximum, 36 detectors will be installed around the sample in a cylindrical arrangement to minimize the dead area. In addition, one detector will be installed underneath the sample to cover qualitatively different reciprocal lattice space from the others. This makes UB matrix more precisely and gives crucial information especially for magnetic structure analyses. The total covered solid angle around the sample will be 4 sr, which enables the efficient measurements and improves the completeness of the data. Schematic drawings of the detectors arrangement are shown in figure 3.
2.4. Sample environment
One of the main aims of SENJU is to pursue precise crystal and magnetic structure analyses under multiple extreme conditions. SENJU is designed to accept various sample environment apparatuses for this purpose. A room temperature apparatus, a standard closed-cycle refrigerator, a 7 T superconducting magnet and a dilution refrigerator will be introduced in the initial stage; one typical “multiple extreme” condition at the beginning is under the magnetic field of 7 T below 50 mK. It is of great importance to reduce background from such apparatuses for the precise structural study. In this respect, unique designs, such as a piezo motor based goniometer inside the cryostat, is employed. In order to realize distinct experimental conditions, installation of an incident neutron polarization device, a high-pressure cell, a high-temperature furnace and a photo-irradiation device is planned as a future upgrade.

3. Construction schedule and current status
The designs of all the devices and the floor layout have been already finished. The devices are manufactured in factories and almost completed. The software to operate the devices from GUI and to perform the data reduction and visualization is also being developed. The data reduction and visualization components of the software are based on STARGazer [6]. Although the construction schedule has been delayed because of the devastating disaster, SENJU will be in commission in 2012.

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