Designing PLANET: Neutron beamline for high-pressure material science at J-PARC

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Abstract. The powder diffractometer dedicated to high-pressure experiments (PLANET) is now being constructed on BL11 at the spallation neutron source of J-PARC. PLANET aims to study structures of hydrogen-bearing materials including dense hydrous minerals of the Earth’s deep interior, magmas and light element liquids. The instrument will realize diffraction and radiography experiments for powder and liquid/glass samples at high pressures up to 20 GPa and 2000 K. It covers d spacing from 0.2 Å to 4.1 Å at 90° bank within the first frame. The design and performance of PLANET have been evaluated using Monte Carlo simulations.

1. Introduction

Neutron diffraction measurement is a useful method to study crystal structure of hydrogen bearing materials, order-disorder transitions of minerals, structure of light element liquids at high pressure, which are difficult to conduct with x-ray experiments. Main obstacle in high pressure experiments is weak signal derived from tiny sample volume and limited opening window of high-pressure device. Material and Life Science experimental Facility (MLF) of Japan Proton Accelerator Research Complex (J-PARC) will be one of the most powerful spallation neutron facilities in the world. The pulsed neutron source with a liquid Hg target is designed to be running at 25 Hz with a power of 1 MW. Such MW class pulsed neutron source will allow us to access unprecedented high-pressure and high-temperature conditions in neutron experiments.

PLANET is one of the neutron diffractometers in MLF and now being constructed on BL11. It is a so-called high-pressure dedicated beamline such as PEARL at ISIS in the UK and SNAP at SNS in the US, and intended to enable large variety of high-pressure experiments. PLANET will realize the measurements of diffraction and radiography for powder and liquid/glass samples at high pressures up to 20 GPa and 2000 K using a large sized multi-anvil hydraulic press that can apply forces of ~1500 ton. Targeted sample volume is a few cubic millimeters. Such large sized presses were installed on the synchrotron radiation beamlines (e.g. Ref. [1]). In addition to installation of the large sized press, the use of three different type of compact high-pressure devices is also planned [2]. Here we present design and performance of PLANET evaluated by Monte Carlo ray tracing using McStas program [3].

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Figure 1. Schematic drawing of the geometry of PLANET instrument.

### Table 1. Specifications of PLANET

| Specification                        | Value                                      |
|--------------------------------------|--------------------------------------------|
| Moderator                            | Decoupled H\(_2\) (para)                  |
| Source to sample (L\(_1\))           | 25 m                                       |
| Sample to detector (L\(_2\))         | 1.5 m                                      |
| Angular coverage                     | horizontal: ±11°, vertical: ±35°           |
| Wavelength range                     | 0.3 - 5.8 Å                                |
| \(Q_{\text{max}}\)                   | 30 Å\(^{-1}\)                              |
| Resolution at 90° bank               | \(\Delta d/d \leq 0.005\)                |

2. Overview of PLANET

PLANET is a neutron diffractometer optimized to observe structures of hydrogen-bearing crystals including hydrous minerals of the Earth’s deep interior, magmas and light element liquids. The performance for the instrument required by users vary according to their research fields such as earth and space science, material science, and high-pressure physics and chemistry. Therefore, the instrumental design should incorporate wide \(Q\) range and have the flexibility for intensity-resolution optimization. Instrumental design was optimized based on the following concepts: (i) coverage of \(d\)-spacing from 0.2 Å to 4 Å in the first frame, (ii) the acceptable instrumental resolution \(\Delta d/d\) should be less than 0.5% at 90° bank; (iii) effective focus of neutrons with wavelengths less than 1 Å using a non-parallel supermirror guide, (iv) trade of resolution for intensity using slits and replaceable focusing devices.

Figure 1 shows the design of the instrument. Main specifications are listed in Table 1. The instrument views a decoupled liquid H\(_2\) moderator which has a cross section of 100 × 100 mm\(^2\). The primary and secondary flight paths are 25 m and 1.5 m, respectively. A total of 7.4-m-long steel collimators are inserted into the shutter and the shield so as to limit beam divergence to natural collimation. 11.5-m-long supermirror guide begins at a distance of 11.5 m from the moderator. Convergent slits are installed at guide entrance and exit in order to limit beam divergence and beam path for high-resolution diffraction measurement and radiography experiment. Sample is placed at 2 m from the guide exit.

Installation of 90° detectors located at 1.5 m from the sample position is planned. For the powder diffraction measurements using a multi-anvil press, an incident neutron beam passes through the vertical anvil gaps and irradiates the sample in the pressure medium. diffracted neutrons go through the other anvil gaps at 90° direction. Accordingly, 90° detectors are well compatible with a multi-anvil press. 290 half inch-\(^3\)He linear position sensitive detectors with 600 mm length will be arranged horizontally and form these detector banks, which cover the scattering angle of \(79° \leq 2\theta \leq 101°\) and \(-35° \leq \varphi \leq +35°\).
for vertical direction from the scattering plane. The detector resolution along the detection of detector wire is estimated to be 5 mm.

Two bandwidth choppers and a $T_0$ chopper are located at 7.1, 10.6 and 10.1 m apart from the moderator, respectively. Bandwidth of $\Delta \lambda = 5.8$ Å is available using 25-Hz pulsed source. This allows diffraction data to be collected for $d$-spacing up to 4.1 Å. Accessible maximum $Q$ value is 30 Å$^{-1}$ using $T_0$ chopper with 50 Hz drive. A wide wavelength range up to about 11 Å can be provided by an operation of the bandwidth chopper at 12.5 Hz.

3. Design of guide

PLANET has a tapered supermirror guide tube for the efficient transportation of the short wavelength neutron ($\sim 0.3$ Å). The preliminary idea of guide design has been given in Ref. [4]. Figure 2 shows the geometry of the guide, which has a rectangular cross-section and which consists of four walls coated with supermirror material. Shape of ellipse is defined by the reflect angle at guide exit and the beam divergence with the acceptable instrumental resolution (0.5% in $\Delta d/d$). In order to obtain large flux for shorter wavelength, it is necessary to keep the reflection angles small less than the critical angle of supermirror coating along the guide. Hence, moderate convergence of the guide is desirable.

Furthermore, focusing neutron beams using a guide increases the incident beam divergence and degrades the instrumental resolution, although the intensity at the sample position is improved. For PLANET, the instrumental resolution is designed to be 0.5% in $\Delta d/d$ in the high-intensity mode. An analytical approximation to the instrumental resolution in $\Delta d/d$ is given by the following expression:

$$
\left( \frac{\Delta d}{d} \right)^2 = \left( \frac{\Delta L}{L} \right)^2 + \left( \frac{\Delta t}{t} \right)^2 + \left( \frac{\Delta \theta}{\tan \theta} \right)^2,
$$

where $t$ is the time of flight, $L$ is the flight path from moderator to sample to detector, and $\theta$ is half of the scattering angle. For the beamline configuration of PLANET and 3 mm diameter sample, accepted incident beam divergence is 5.3 mrad for $\Delta d/d$ of 0.5% at 90° bank and contribution of incident beam divergence to instrumental resolution is 0.4 %. Therefore cross section of guide exit located at 2 m apart from the sample position should be $21 \times 21$ mm$^2$. Cross section of the guide entrance is determined from natural collimation. Gap in the angular divergence would appear and lower the beam intensity when the cross section exceeds this value.

![Figure 2. Geometrical condition of PLANET neutron guide.](image-url)
Design of elliptical geometry is optimized by means of incorporating several different grade mirrors [5] and linear approximation with planar guide in order to save cost for production without degradation of the intensity performance. Figure 3 shows the simulated flux gains for a guide with $m=3.7$ coating and elliptical shaped curve (ideal guide) and a guide with $m=2.5-3.7$ coating and linearly approximation as shown in Fig.2 (practical guide), respectively. Gain factors are calculated from intensities spatially integrated over $3 \times 3 \text{ mm}^2$ at sample position with respect to that of a natural flight path of 25 m. The practical guide designs exhibit the gain of about a factor of 6 above wavelength of 0.5 Å. The gain factor decreases rapidly with decreasing wavelength below 0.5 Å and is unity at 0.2 Å. This is due to the lowering of reflectivity of mirror and the decreasing beam divergence caused by small critical angle in shorter wavelength. The intensity with the practical guide design is identical to that with the ideal guide design above wavelength of 0.3 Å, thus no significant degradation of the performance is observed within the instrument’s wavelength range by replacing of mirror coating and linearly approximation.

### 4. Instrumental performance

PLANET is designed to have two configurations for diffraction measurement: high-intensity mode and high-resolution mode. The instrumental resolution can be controlled effectively by varying the horizontal divergence of the incident beam using the slit 2 because contribution of the slit 2 width to angular uncertainty is large compared to the sample size and the detector resolution.

Figure 4 shows the simulated diffraction profiles for 222 reflection of Si powder obtained from high-intensity mode and high-resolution mode. Here, widths of the slit-2 in high-resolution mode and high-intensity mode are 5 mm and 21 mm respectively. Sample size is 3 mm diameter. The results show that symmetric profile shapes for both configurations. The high resolution mode achieves resolution 0.25% in $\Delta d/d$. In the high intensity mode, a resolution calculated from a simulated profile is 0.53% in $\Delta d/d$ and shows good agreement with the resolution delivered using Eq. (1). The integrated intensity gain as a result of increasing horizontal divergence is 5. Since timing resolution calculated from the moderator pulse shapes is an almost constant, the both configurations show flat resolution dependence on $d$ spacing.

The incident neutron fluxes on the sample position in the first frame (0.3 – 5.8 Å) are $9.6 \times 10^7$ n/s/cm$^2$ in high-intensity mode and $2.0 \times 10^7$ n/s/cm$^2$ in high-resolution mode when the neutron source operates at 1 MW. Using compact focusing devices [6–9] and increasing vertical divergence incident on the sample, neutron flux will be further improved without sacrificing the instrumental resolution.

One of the most critical issues with high pressure neutron experiments is the neutron illumination...
Figure 4. Simulated diffraction profiles of Si 222 reflection obtained from the high-resolution mode with 5 mm slit 2 width (solid circle) and the high-intensity mode with 21 mm slit 2 width (open circle). Sample diameter and height are both 3 mm.

of the surrounding gasket and cell assembly such as pressure mediums and heaters. Thus the fine collimations for both incident and scattered beams will be crucial for improvement of the signal/background ratio. We are planning to install pinhole collimator and/or compact focusing device near the sample in order to produce a beam spot below the sample size of a few square millimeters. In addition, radial collimators [10–12] will be placed between the sample and the detectors to restrict the field of view of the detectors to the sample volume and eliminate background scattering from the surrounding materials right next to the sample. To collimate beams more effectively, using BN anvils that provide self collimation is also considered.

5. Conclusion
Instrument design of high-pressure neutron diffractometer at J-PARC, PLANET, was reviewed. The results of Monte Carlo simulation show that PLANET realizes instrumental resolution, \(\Delta d/d\), of 0.53% in high-intensity mode and of 0.25% in high-resolution mode, respectively. We can obtain large gain above wavelength of 0.3 Å using the optimized supermirror guide. Therefore, PLANET will enable us to explore structure of both liquid and crystal at high-pressure condition with high efficiency. The construction of the instrument started in April 2009 and is scheduled to be completed by April 2011.

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