The HANARO neutron reflectometer with horizontal sample geometry

Chong Oh Lee, a Kwanwoo Shin*, a Jeong Soo Lee, b Chang-Hee Lee, b Sang Jin Cho, b Kwang Pyo Hong, b a Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, Oryong-dong, Buk-gu, Gwangju, 500-712, Korea, kwshin@gist.ac.kr

b HANARO Utilization Technology Development Division, Korea Atomic Energy Research Institute,

P. O. B. 105, Yuseong, Daejeon, 305-600, Korea

1. Introduction

Recently, due to increased interest of Biotechnology (BT) and Nanotechnology (NT), measurement techniques for the interface characterization of the thin film structure and depth profiling are known to be extremely important. In fact, nanosize measurement and characterization techniques are mainly targeting development of the instruments for measurement method of nano structured materials, atomic/molecular structures and magnetic/chemical/physical characterization. Reflectivity measurement, which is located in center of these divisions, is a powerful technique for the study on surfaces and interfaces of materials due to its high spatial resolution perpendicular to the surface.^{1,2} Most of the reflectometers now in Korea have a vertical-sample geometry, and, as a result, are suitable only for solid samples.³ Hence, a reflectometer with a horizontal-sample geometry is currently in great demand for various frontier researches in Korea. Thus, if a neutron liquid spectrometer is constructed in HANARO then will it be a popular instrument for liquid samples.

In this paper, preliminary conceptual designs for the new reflectometer with a horizontal sample geometry at the ST3 thermal port of HANARO (REF-H), and a MCSTAS simulation for the cold source-based reflectometer (BIO-REF) are addressed. The most important concern is the re-installation of the machine, which was originally designed for the HFBR and utilized for several years, and to adapt its functions to maximize its capabilities under the specific environment of HANARO.

2. Characteristics of the BNL H9-A Reflectometer⁵

The BNL reflection spectrometer was originally designed to use 2 monochromators and one deflector crystal (M3), due to the floor space constraints at BNL. Therefore, it will be a challenge, for us to modify this geometry to avoid a significant reduction in intensity during multiple reflections. For the thermal source-based reflectometer (REF-H) at HANARO, the use of three mirror system is inevitable, due to the similar problem to H9-A. However, the first two monochromators can be easily avoided when the dedicated neutron guide is installed for BIO-REF. The intensity at the M3 crystal will be then increased to orders of magnitude of what the intensity of the BNL instrument was by removing those first two monochromators.⁵

The sample stage, translating vertically as q varies, and an active anti-vibration table were not shipped to HANARO. Therefore, a heavy-duty sample table will be needed to support the sample environment with the z-axis translation. For alignment of the sample into the beam, a 2-axis goniometer for a solid sample orientation, and a piezo-elecric anti-vibration system will be installed for liquid surfaces.

Category	Specification	Resolution
Neutron	1.51 Å ⁻¹	
Wavelength		
Working Q range	0.002-0.2 Å ⁻¹	
Sample Size	<40cm	
Deflector	Angular range	0.001°
Crystal(M3)	+1/-5°	
Slit (S3 and S4)	Maximum opening	0.01mm
	5mm	
Sample Table	Vertical travel	0.02mm
	300mm	
Slit(S5)	Maximum opening	0.01mm
	5mm	
Detector(D2)	Vertical travel	
	300mm	0.02mm/0.001°
	Angular range +5°	

Table. 1 Specification of HANARO Reflectometer

3. MCSTAS Simulation for relocation performance with horizontal sample geometry

Since the H9A BNL reflection spectrometry will be installed initially at the ST3 beam port with a thermal source, simulation for the thermal source was performed using the MCSTAS software. In order to optimise the optical performance when it is transferred to a cold source, more extensive simulation together with a design of cold guide was performed and compared.

The thermal neutron spectrum follows a standard Maxwellian distribution at 320K. A thermal source having a radius of 10 cm was designed, which sends neutrons towards, a 16 cm \times 16 cm wide aperture at the edge of the reactor. Total beam flux was set to 5 \times 10¹³ n for the MCSTAS simulations. The source slits, S1 and S2 were placed at distances of 1.5 m and 3.4 m from the source, with 6.2 cm \times 12.0 cm wide and 8.6 \times 18 cm wide apertures respectively. We obtained a total neutron intensity of 4.6 \times 10¹¹ and an effective intensity of 3.0 \times 10⁹ at a wavelength of 2.52 Å after horizontal collimation. The side view of REF-H at the ST3 is shown schematically in Fig. 1.

A flat PG monochromator having 4 (h) x 6 (w) cm was mounted at 6 m from the source (Fig. 1(3)). The mosaic spreads for X and Y direction were fixed to 24". Due to the concrete shielding housing built before the planning of REF-H, the only option for obtaining a monochromated beam out of the shielding housing is to shift the beam 22 cm higher in a parallel configuration using the double monochromators. The second PG monochromator with dimensions of 4 (h) × 6 (w), cm was mounted 31 cm from the 1st monochromator (Fig. 1(4)).

1 cm long graphite filter was installed immediately after the 2^{nd} monochromator. Finally, the beam deflecting mirror



Fig. 1 The layout of REF-H set-up at the ST3 beam port

will be mounted at the same position, where the M3 deflector crystal of the H9-A instrument is located. Due to the limited neutron flux, a m = 3 supermirror was suggested, and provides 90% of the reflection up to 0.063 Å⁻¹, which is equivalent to an incoming q of 0.126 Å⁻¹ at the sample. Two identical beam-defining slits were mounted. The 1st slit (Fig. 1(7)) was located 25 cm from the 2nd monochromator, while the 2nd slit (Fig. 1(8)) was located 95 cm from the 2nd monochromated beam distribution is 2.52 Å, defined by two successive slits, and measured at the sample position.

The overall performance of the REF-H was evaluated by collecting the total intensity (I_t) while the M3 mirror was deflecting progressively. A total intensity of 10^6 out of 5 \times 10^{13} and the neutron flux of 10^5 n cm²/s were obtained up to q = 0.1 Å⁻¹, and the orders of total intensity decayed dramatically at q > 0.12 Å⁻¹. This is, because the M3 mirror cannot deflect above its critical q of 0.063 Å⁻¹. The maximum q can be extended, when REF-H is transferred to the cold source. A cold guide, having a dimension of curved length of 25.5 m and straight length of 22.1 m from the source, with 5 cm (w) \times 1.0 cm (h) was currently planned for the BIO-REF. Operation with a fixed wavelength of 4.6 Å and single monochromater (instead of 3 mirrors for thermal case), then readily give the spectrometer a nominal q-range extending from 0 to 0.21 Å⁻¹. For liquid surfaces, a practical upper-q limit of 0.2 Å⁻¹ should be sufficient.⁶



Fig. 2 3D neutron trajectory simulated by MCSTAS

4. Conclusion

A new neutron reflectometer with horizontal sample geometry is under construction at a thermal neutron port at HANARO, the 30MW research reactor at KAERI. It was originally designed and operated at the H9-A beam port at Brookhaven National Laboratory (BNL), and was relocated to HANARO in 2004. It will be initially installed at the ST3 thermal neutron port without any significant modification, and improvements in structure and performance are planned when the new cold source is installed in 2008. If successfully installed, it will be the first reflectometer in Korea for the study of free surfaces, which is currently lacking. The feasible wavelength of incident neutron beam is 2.52Å and this would permits the q-ranges up to 0.12 Å⁻¹ for the thermal source. For the cold source, the q-range will be extended to 0.21 Å⁻¹.

5. Acknowledgement

We thank JY Soh of KAERI for the help of MCSTAS simulation. This work was sponsored by National Research Laboratory and Basic Atomic Energy Research Institute..

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