

## Upgrade of the Wide-Angle Neutron Diffractometer at the High-Flux Isotope Reactor

Yoshinobu ISHII, Susumu KATANO, Jun-ichi SUZUKI, Kazuya AIZAWA, H. Ray CHILD,<sup>1</sup>  
Yukio MORII and Jaime A. FERNANDEZ-BACA<sup>1</sup>

*Advanced Science Research Center, Japan Atomic Energy Research Institute, Ibaraki 319-1195, Japan*

<sup>1</sup>*Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6393, USA*

The Wide-Angle Neutron Diffractometer (WAND) installed at the High-Flux Isotope Reactor (HFIR) has been upgraded for new experiments. The main feature of this upgrade is the replacement of its detector with a newly developed curved one-dimensional <sup>3</sup>He position-sensitive counter composed of 624 individual anodes. From the results of test-measurements of the detector performance, it is found that the intrinsic angular resolution and the maximum neutron-counting rate per anode are 0.25 degrees and  $2.0 \times 10^5$  counts/second, respectively.

KEYWORDS: flat-cone geometry, one-dimensional position sensitive detector, WAND

### §1. Introduction

The Wide-Angle Neutron Diffractometer (WAND) was installed at the HB-4 port of the High-Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL) in the middle of 1980's under the neutron scattering cooperative program between Japan and USA.

This diffractometer is a unique instrument in the neutron scattering field because it can measure the intensity of neutrons diffracted from a single crystal under the flat-cone configuration, and the intensity from a powder sample or a poly-crystal sample over a wide diffraction angle at a time. The WAND has been mainly used for diffuse-scattering experiments in single crystals, and for time-slice measurements of phase transition kinetics of powder samples or poly-crystals.<sup>1)</sup>

The upgrade of the WAND is a response to the increasing demand for higher performance as new challenging physical problems (like the physics of the strongly correlated electron systems) emerge. The main part of this upgrade is the replacement of its one-dimensional position-sensitive <sup>3</sup>He detector with a newly developed state-of-art counter. In this paper we show the performance of the new WAND. Before this upgrade, we made a small proto-type detector and carried out a performance test.<sup>2)</sup>

### §2. Instrumentation

#### 2.1 The new WAND

The new detector at the WAND is a curved one-dimensional position sensitive counter consisting of 624 individual anodes and their associated electronics. These anodes are arranged at 2 mm steps from each other, which correspond to 0.2 degrees of the diffraction angle. The detector covers about 125 degrees. The WAND and the detector are shown schematically in Fig. 1. Since the sample table and the detector are able to be tilted up to 45 degrees as shown in Fig. 1(a), we can measure the diffraction intensities not only in the basal plane as in

most diffractometers, but also in higher scattering planes (flat cone geometry).

#### 2.2 Test measurement for specification

A set of standard powder samples, a perfect Si-single crystal and a pyrolytic graphite crystal were used to check the performance of the new WAND. Before the

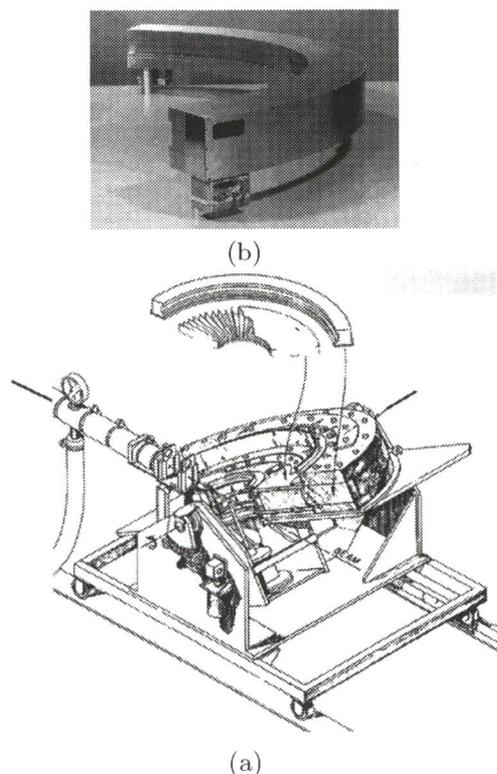


Fig.1. A schematic illustration of the WAND(a) and a photograph of the curved one-dimensional position sensitive detector(b). The sample stage and the detector can be tilted up to 45 degrees from the horizontal plane. The detector covers about 125 degrees in diffraction angle.

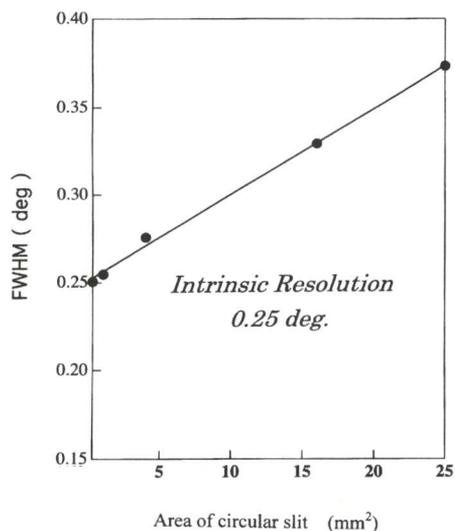


Fig. 2. The full width at a half maximum (FWHM) of the 220 Bragg line reflected from a perfect Si-single crystal as a function of the area of the slit. The intrinsic resolution of the detector is 0.25 degrees, which is obtained by extrapolating to the zero slit.

experiment we checked the counting uniformity of the detector by using a vanadium rod and also checked the uniformity of the arrangement of anodes by measuring the Bragg reflection lines diffracted from the standard powder samples. The diffraction angle has a linear relationship with anode number over a wide range of diffraction angles as  $\text{Ang} \propto 0.2000(\pm 0.0001)\text{Ch}$ , where Ang and Ch mean the diffraction angle and the anode number, respectively.

To estimate the intrinsic angular resolution of the detector, the full width at half maximum (FWHM) of the 220 reflection line diffracted from a perfect Si-single crystal was measured by changing the diameter of a circular slit at the incident neutron beam. The FWHM of the reflection lines as a function of area of the slit is shown in Fig. 2. From this figure, the intrinsic angular resolution of the detector is extrapolated to 0.25 degrees.

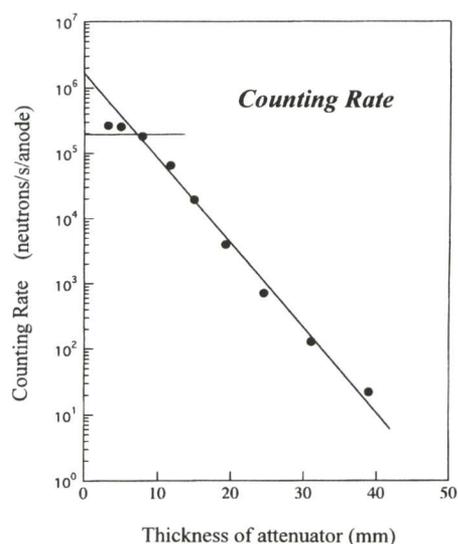


Fig. 3. The counting rate of the detector as a function of thickness of the attenuator. (See text)

To evaluate the maximum counting-rate of this detector, intensity measurements of the 002-reflection line diffracted from a graphite crystal were carried out by changing the thickness of an attenuator placed in the incident neutron beam. Figure 3 shows the counting rate as a function of thickness of the attenuator. From this figure, one can see that the neutron counting rate has a linear relationship with the attenuator thickness up to  $2 \times 10^5$  counts/second per anode. Above this value, the counting rate was deviated from an extrapolated line. Thus the maximum counting of this detector is  $2 \times 10^5$  counts/second.

A typical diffraction pattern of a standard Si-powder sample of about half gram is shown in Fig. 4. The cross symbol indicates the measured data. The solid, dotted and broken lines indicate the results of the Rietveld refinement,  $\Delta d/d$  and the line width of the diffraction line, respectively. The resolution of the WAND used as a powder diffractometer is about 2% in the range above of

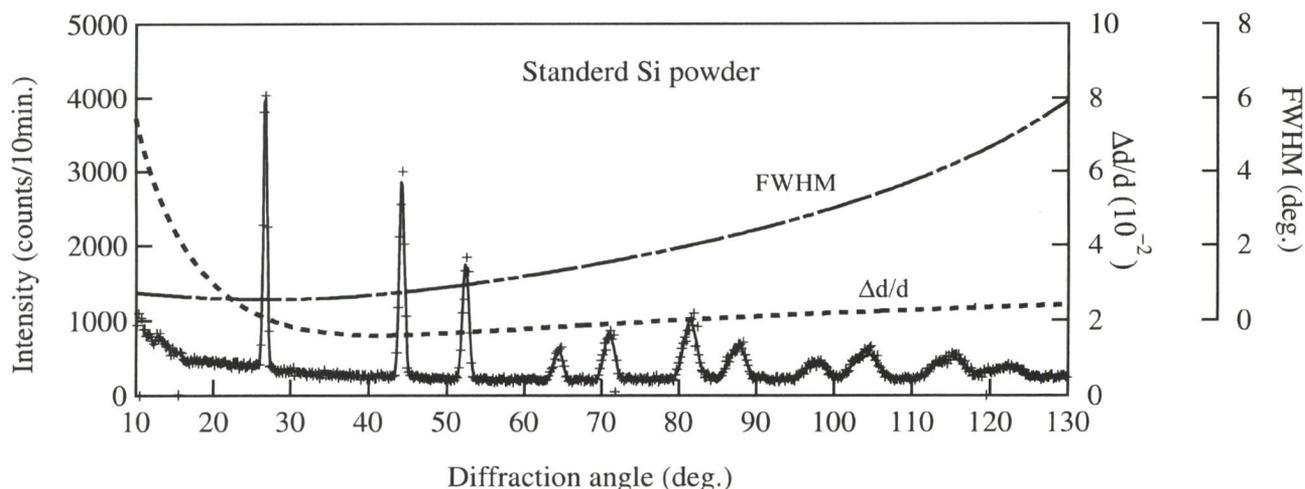


Fig. 4. Diffraction pattern of standard Si-powder sample of a half gram. The solid line shows the result of the Rietveld refinement. The broken and dotted lines show the line width of the diffraction line and the resolution in  $\Delta d/d$  as a function of diffraction angle, respectively.

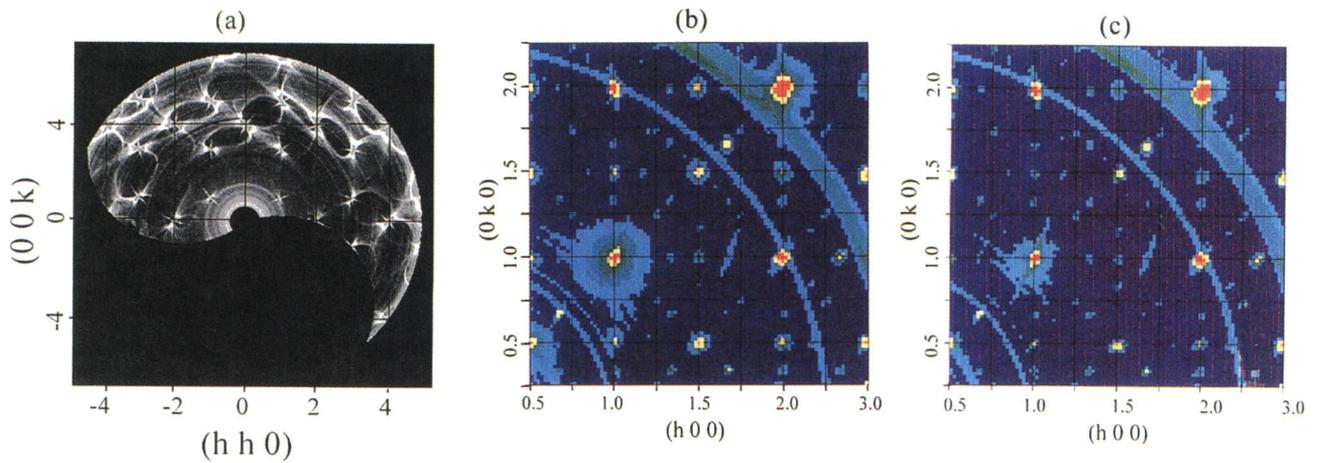


Fig.5. Contour maps of neutron intensity diffracted from single crystals.

diffraction angle between 30 and 130 degrees. The line width for the reflection line is about one degree around of 25 degrees in diffraction angle. This line width gradually increases

with increasing diffraction angle and is about 6 degrees at the diffraction angle of 130 degrees. From this figure one can see that the neutron counts for the Bragg peaks are high, despite the small sample and the short counting rate. Therefore the WAND is very suitable for the time-slice measurement for studies such as phase transition kinetics.

### 2.3 Demonstrations for single crystal measurements

Several studies of strongly correlated electron systems using the new WAND have already been performed.<sup>3-5)</sup> Here we show miscellaneous experimental results for demonstration purpose.

In Fig.5 we show the 2-dimensional diffraction patterns of two single crystals. Figure 5(a) shows the diffraction intensity for a Si-single crystal set the  $[1\bar{1}0]$  crystal axis perpendicular to the scattering plane. The measurement was conducted by stepping the sample around the  $[1\bar{1}0]$  axis. The step and the counting period for each scan were 0.2 degrees and 90 sec., respectively. Since the detector has a high performance in counting rate and resolution as mentioned above, some patterns due to phonons are clearly observed around at Bragg peaks.<sup>6)</sup>

Contour maps for  $(\text{Pr}_{0.7}\text{Ca}_{0.3})\text{MnO}_3$  at 40 K under a magnetic field of 0 T and 5 T are shown in Fig.5(b) and (c), respectively.<sup>7)</sup> From these figures, one can see that the diffuse scattering pattern observed around at the Bragg points of (110) and (220) shrink and grow to ferromagnetic peaks by applying an external magnetic field. This shows that most of the ferromagnetic clusters

at zero magnetic field grow to become part of a homogeneous infinite ferromagnetic clusters when a magnetic field is applied. As shown above, the new WAND is very useful for observations of the diffuse scattering in a short measuring period over a wide range of the reciprocal space.

The upgrade of the HFIR will be completed by the end of 2001. After the HFIR upgrade, the WAND will be installed at the HB2 port and the incident neutron beam intensity will be increased by a factor of 5 ~ 10 compared with the present set up.

### §3. Summary

The specifications of the new WAND are as follow:

- 1) The intrinsic resolution is 0.25 degrees.
- 2) The maximum counting rate per anode is  $2.0 \times 10^5$  counts/second.
- 3) The resolution ( $\Delta d/d$ ) is 1.7 % around the scattering angle of 35 degrees.

This work was supported by JAERI and ORNL under the JAERI-DOE cooperative program on neutron scattering. ORNL is managed by UT-BATTELLE, LLC (UT-BATTELLE) for the US DOE under contract number DE-AC05-00OR22725.

- 
- 1) Progress report on JAERI-ORNL cooperative neutron scattering research I-IV (1985, 1987, 1993 and 1996).
  - 2) S. Katano *et al.*: Physica B **241-243** (1998) 198.
  - 3) J.A. Fernandez-Baca *et al.*: J. Phys. Soc. Jpn. **70** (2001) Suppl. A. 85
  - 4) P. Dai *et al.*: Phys. Rev. Lett. **85** (2000) 2553.
  - 5) Y. Yamada *et al.*: Phys. Rev. B **62** (2000) 11600.
  - 6) N. Wakabayashi *et al.*: Physica B **241-243** (1998) 320.
  - 7) S. Katano *et al.*: Physica B **276-278** (2000) 786.