

ICANS XIX,  
19th meeting on Collaboration of Advanced Neutron Sources  
March 8 – 12, 2010  
Grindelwald, Switzerland

**SANDWICH TYPE DISPERSIVE MONOCHROMATORS BASED ON  
CYLINDRICALLY BENT PERFECT CRYSTALS (BPC)**

P. MIKULA  
*NUCLEAR PHYSICS INSTITUTE ASCR, V.V.I. AND RESEARCH CENTRE REZ, LTD.,  
250 68 ŘEŽ, CZECH REPUBLIC*

M. VRANA, J. SAROUN  
*NUCLEAR PHYSICS INSTITUTE ASCR, V.V.I., 250 68 REZ, CZECH REPUBLIC*

M. FURUSAKA  
*HOKKAIDO UNIVERSITY, KITA-KU, SAPPORO 060- 8628, JAPAN*

AND

B.S. SEONG, M.K. MOON  
*KAERI, 1045 DAEDOK-DAERO, YUSEONG-GU, DAEJEON, REPUBLIC OF KOREA*

**ABSTRACT**

Dispersive multiple reflections realized by means of two BPC slabs of different cut used as a sandwich can provide a monochromatic beam of excellent resolution parameters. The dispersive sandwich monochromator/analyzer provides a freedom to combine crystal slabs of different cuts i.e. different crystal reflections for the double diffraction process. Therefore, by a suitable combination of two slabs, one can obtain monochromatic neutron beam of any wavelength in the thermal region. Depending on the bending radius of the sandwich the resolution  $\Delta\lambda/\lambda$  and the  $\Delta\alpha$  collimation can be continuously adjusted in the range of  $5 \times 10^{-5}$  -  $1 \times 10^{-3}$ . Of course, that such dispersive BPC elements can be used also for the high-resolution analysis of the scattered beam as well as for a high precision  $\lambda$ -calibration of the TOF neutron scattering devices.

**1. Introduction**

In many cases, new samples and necessity of measurement of finer effects require a substantial increase of angular and/or energy resolution of conventional diffractometers operating in a conventional performance mode. In such a case, a convenient monochromator plays a key role. Bent perfect crystal (BPC) slabs as neutron monochromators have been already proved as an excellent alternative of conventional mosaic crystals. They provide a way how to increase luminosity and angular/energy resolution of some scattering devices installed usually at steady state sources [1,2]. An increase of the luminosity is carried out by focusing in real space, while a higher resolution can be achieved by focusing in momentum space and by a rather small effective mosaicity of the BPC elements. However, in the case of TOF scattering devices, the BPC elements practically have not been used and with respect to the TOF techniques the Bragg diffraction optics is far from being fully explored. New possibilities of more effective use of neutron scattering devices have recently opened an employment of sandwich type BPC

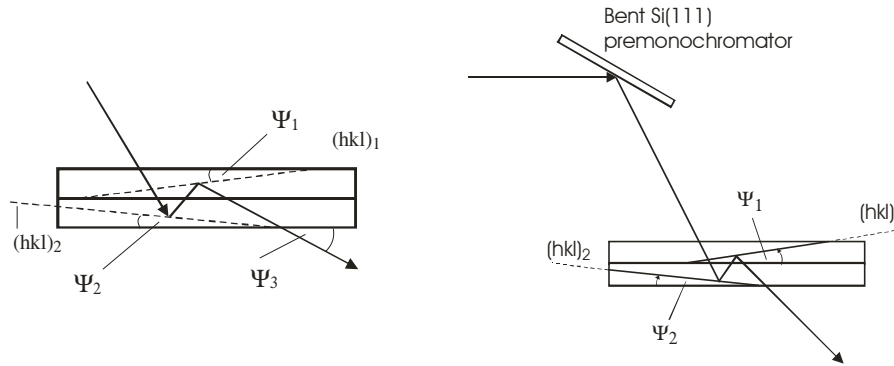


Fig. 1. (a) - schematic diagram of a two-step double reflection process realized by two independent slabs put together in the form of a sandwich and (b) - the experimental arrangement used for testing.

monochromators. They provide e.g. multiple wavelength monochromatized beams [3] and a larger range of curvatures permitting an easier luminosity and resolution optimization of some dedicated instruments [4,5]. Together with construction of new powerful neutron sources, new scattering instruments with improved resolution properties are designed. One of the candidates of monochromators for very high resolution neutron diffractometers and spectrometers appear so called dispersive monochromators based on a dispersive double diffraction process. It can be realized by means of two independent crystals [6,7] or by exciting a strong multiple reflection effect inside one elastically deformed perfect crystals [7-10]. However, recently it has appeared that the dispersive double diffraction process can be realized by means of a sandwich using two bent perfect crystal slabs of a different cut (see Fig. 1). The choice of the crystal cut provides a freedom in combination of slabs in the sandwich as well as the reflections involved. Then, the choice of the reflections and the corresponding angles  $\Psi_1$  and  $\Psi_2$  determine the neutron wavelength and the final monochromator take-off angle  $2\theta_M = \Psi_3$ . In this contribution we present the results of test experiments with such dispersive monochromators.

## 2. Choice of the crystals and the experimental tests

Depending on the cut of the crystal slabs one can use many combinations of two reflections realized by the sandwich. For example, the sandwich with the first slab having the main face parallel to the planes (110) and the longest edge parallel to the vector [1-11] and the second slab having the main face parallel the planes (11-1) and the longest edge parallel to the vector [112] provides the following reflection combinations:

$$\text{Si}(220) (\Psi_{220}=0^\circ) + \text{Si}(331) (\Psi_{331}=-22.00^\circ) \quad \theta_{220}=31.39^\circ \quad \theta_{331}=51.39^\circ \quad \lambda=0.20 \text{ nm}$$

$$\text{Si}(220) (\Psi_{220}=0^\circ) + \text{Si}(33-1) (\Psi_{33-1}=-48.53^\circ) \quad \theta_{220}=40.45^\circ \quad \theta_{33-1}=88.98^\circ \quad \lambda=0.25 \text{ nm}$$

Similarly, the sandwich with the first slab having the main face parallel to the planes (111) and the longest edge parallel to the vector [11-2] and the second slab having the main face parallel the planes (11-2) and the longest edge parallel to the vector [111] provides another two alternatives:

$$\text{Si}(111) (\Psi_{111}=0^\circ) + \text{Si}(111) (\Psi_{111}=-29.50^\circ), \quad \theta_{111}=75.25^\circ \quad \lambda=0.606 \text{ nm}$$

$$\text{Si}(111) (\Psi_{111}=0^\circ) + \text{Si}(11-1) (\Psi_{11-1}=-29.50^\circ), \quad \theta_{11-1}=14.75^\circ \quad \lambda=0.160 \text{ nm}$$

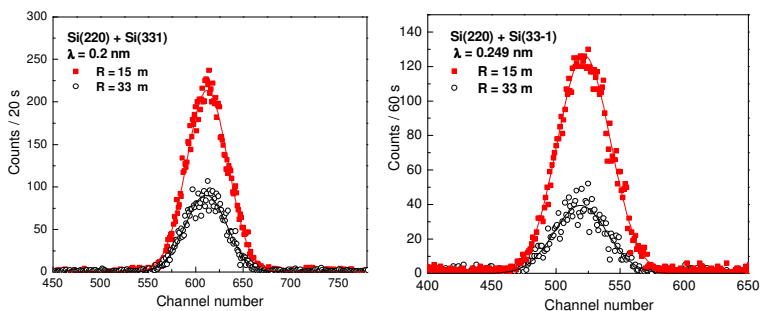


Fig. 2. The double reflected neutron beam as seen by 1-d PSD for two different radii of curvature  $R$  of the sandwiches.

curvature of 12 m, the double-reflection process was verified with different sandwiches situated at the sample position. As at our diffractometer we were limited by a maximum take-off angle of  $60^\circ$ , using Si(111) premonochromator provided us a large range of wavelengths of monochromatic neutrons (see Fig. 1b). Then, the double diffracted beam was registered and its profile imaged by a linear position sensitive detector (1d-PSD). It can be seen from Fig. 2 that as expected, the intensity of the double reflected beam strongly depends on the radius of curvature of the sandwich. It should be pointed out that in the case of the Si(4-40) reflection, the Bragg angle  $\theta_{440}=61.22^\circ$  but the take-off angle  $\Psi_3=70.46^\circ$ . Similarly, in the case of the Si(33-1) reflection, the Bragg angle  $\theta_{331}=88.98^\circ$

Experimental test of the sandwich type dispersive monochromator was carried out in two steps. First, by using a bent Si(111) premonochromator of the dimensions of  $200 \times 40 \times 4 \text{ mm}^3$  (length  $\times$  width  $\times$  thickness) and of the radius of

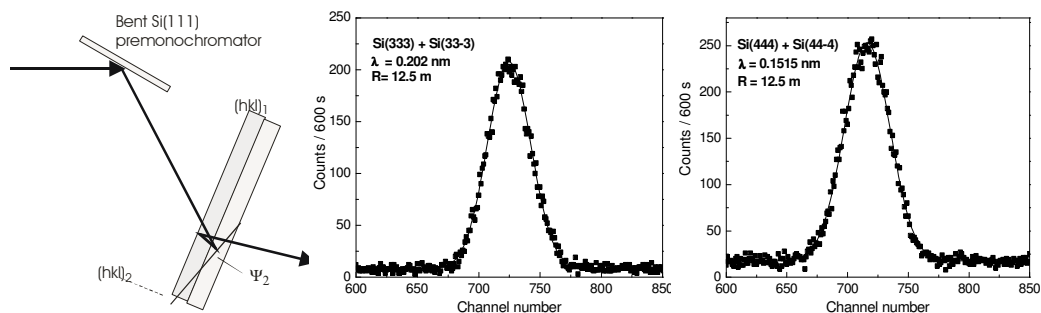


Fig. 3. Schematic diagram of the experimental performance and the experimental results related to the double reflected neutron beam as seen by 1-d PSD related to the third and fourth order neutrons with respect to the first order.

(notice back-scattering diffraction geometry) but the take-off angle  $\Psi_3=97.06^\circ$ . Then, we tested the the sandwich with dispersive combination of Si(111) reflections. However, the first combination with  $\theta_{111}=75.25^\circ$  requires the neutron wavelength of 0.606 nm which was not accessible at our thermal polychromatic beam, the test experiment was carried out with the third ( $\lambda=0.202 \text{ nm}$ ) and fourth order ( $\lambda=0.1515 \text{ nm}$ ) neutrons on Si(333) and Si(444) planes, respectively. The obtained results are shown on Fig. 3. Even though  $\theta_{hhh}=75.25^\circ$ , the take-off angle is only  $\Psi_3=59^\circ$ . The same sandwich permitted also performance for the wavelength of 0.16 nm, however, with much stronger detector signal (see Fig. 4). Also in this case the take-off angle is  $\Psi_3=59^\circ$ .

Finally, as the second step, the sandwich combination Si(111)+Si(11-1) from Fig. 4 was situated at the monochromator position and the obtained monochromatic beam was used for studies of collimation properties of the monochromatic beam for different radii of curvature of the sandwich. Two slits of the width of 1 mm and separated by 10 mm were put into the obtained monochromatic beam and the intensity profile of the passed neutrons were registered by one dimensional position sensitive detector having rather poor spatial

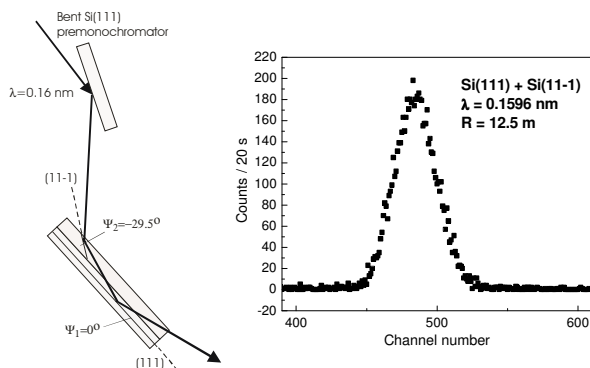


Fig. 4. Schematic diagram of the experimental performance and the obtained experimental result.

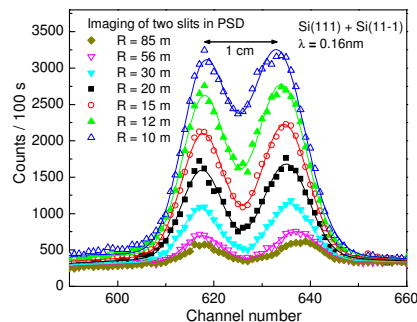


Fig. 5. A beam from the sandwich monochromator passing through two slits of the width of 1 mm as registered by 1d-PSD at the distance of 70 cm.

resolution of about 4 mm. Nevertheless, a high collimation of the monochromatic beam was proved. After that by using such highly collimated and monochromatic beam diffraction on Fe-single crystal as a sample has been carried out. Fig. 6 shows examples of the rocking curves of a Fe(110)-single crystal with respect to this sandwich monochromator. It is clearly seen from the Fig. 6 that the resolution depends on the sandwich curvature and for the larger bending radius of 30 m (i.e. for higher resolution) one can distinguish presence of two slightly misoriented mosaic blocks. Therefore, the obtained rocking curves were fitted by two Gaussians and thus provided two values of FWHM related to individual mosaic blocks. In this case the angular resolution was of the order of  $5 \times 10^{-4}$ .

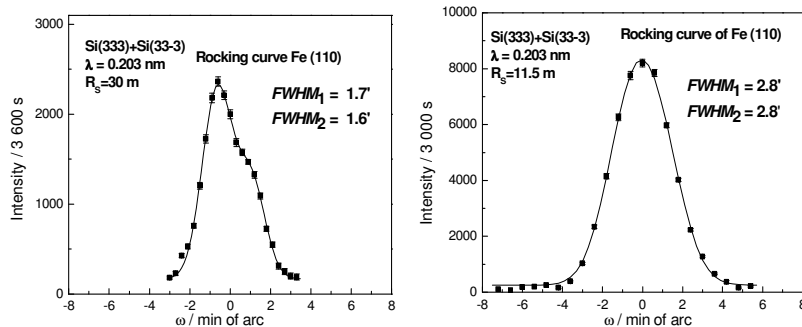


Fig. 6. Two examples of the rocking curves of Fe(110) single-crystal with respect to the dispersive sandwich monochromator for two different values of the bending radius.

However, the higher angular resolution (for a larger bending is adjusted, the lower detector signal will be obtained. Similar results were also obtained with other combinations of the crystal slabs in the sandwich which we had at a disposal.

### 3. Conclusion

The presented results clearly demonstrate the feasibility of using double reflection effects realized by means of the two-slab-sandwich for high resolution monochromatisation (or analysis) of neutrons. For minimizing resolution and maximizing the peak intensity a special care should be paid to a proper alignment of the monochromator slab with respect to the incident beam axis and the scattering plane. As was demonstrated, the obtained intensity of the monochromatic beam as well as provided resolution depend on radius of curvature of the sandwich. Furthermore, also other parameters play important role: asymmetry of diffraction geometry of individual crystals as well as of the whole sandwich, the neutron wavelength and the lattice planes involved.

ICANS XIX,  
19th meeting on Collaboration of Advanced Neutron Sources  
March 8 – 12, 2010  
Grindelwald, Switzerland

Of course, that the neutron current provided by such dispersive monochromator corresponds to intersection of two phase-space elements corresponding to individual reflections. For finding sufficiently strong dispersive double-reflection effects suitable for high-resolution diffraction studies i.e. for finding optimum parameters of the crystal slabs in the sandwich as well as for an optimum design of the scattering device, Monte Carlo simulations would be desirable. The advantages of dispersive sandwich monochromator can be summarized as: one instrument axis for the double reflection process, a high  $\Delta\lambda/\lambda$  and the angular resolution, a rather small take-off angle of the monochromator, a large Bragg angle (at least) of one reflection and good peak reflectivity of the bent perfect crystals. In the extreme case, one can work with the back scattering resolution on a conventional instrument with a rather small take-off angle.

#### 4. Acknowledgements

Bragg diffraction optics investigations are in the Czech Republic supported by the projects MSM2672244501, AVOZ104805505, ASCR-M100480901 and GACR P204/10/0654.

#### 5. References

1. M. Popovici, and W.B. Yelon, *J. Neutron Research* **3** (1995) 1.
2. P. Mikula, V. Wagner, and M. Vrana, *Physica* **B283** (2000) 289.
3. M. Vrana, P. Mikula, P. Lukas, and V. Wagner, *Physica B*, **241-243** (1998) 231.
4. J. Kulda, and J. Saroun, *Nucl. Instrum. Methods A* **379** (1995) 155.
5. P. Staron, H.U. Ruhnau, M. Mamotti, P. Mikula, and R. Kampmann, *Physica B* **276-278** (2000) 158.
6. P. Mikula, M. Vrana, V. Wagner, Y.N. Choi, S.A. Kim, H.S. Oh, K.H. Sung, and C.H. Lee, Proc. of Int. Conf. ATEM'03, September 10-12, 2003, Nagoya, Japan. CD ROM Published by The Japan Society of Mechanical Engineers No. 03-207, Sep. 9, 2003, paper OS04W0288.
7. P. Mikula, M. Vrana, M. Furusaka, V. Wagner, Y.N. Choi, M.K. Moon, V.T. Em, and C.H. Lee, *Nucl. Instrum. Methods in Phys. Research*, **A529** (2004) 138.
8. P. Mikula, R.T. Michalec, M. Vrana, and J. Vavra, *Acta Cryst.* **A35** (1979) 962.
9. P. Mikula, M. Vrana, and V. Wagner, *Physica B*, **350** (2004) e667.
10. P. Mikula, M. Vrana, and V. Wagner, *Zeitschrift für Kristallographie*, Suppl. **23** (2006) 205.