Applied strain effect to the luminosity and divergence of neutron monochromator with fully asymmetric diffraction

M R Muslih\textsuperscript{1}, R Apriansyah\textsuperscript{1} and Mikula\textsuperscript{2}

\textsuperscript{1}Neutron Scattering Lab, Center for Science and Technology of Advanced Materials, Gd. 40 Kawasan PUSPITEK Serpong Tangerang
\textsuperscript{2}Neutron Physics Institute, ASCR, v.v.i. CZ – 250 Rez, Czech Republic
E-mail: rifai@batan.go.id

Abstract. The effect of applied strain on the luminosity and divergence of neutron monochromator with fully asymmetric diffraction geometry will be reported. The monochromator used silicon single crystal with 200 x 30 x 4 mm\textsuperscript{3}, which has the parallel face of the crystal to the planes (220). The plain used for this monochromator was (311), which has a 31.5 degree to the (220) face. Fully asymmetric diffraction geometry had been fulfilled with the take-of-angle of the monochromator at 63 degrees. Four lines are bending system used for applying the strain to the crystal, which remote-controlled by computer. The 0, 25, 50, 75, 100, 125, 150, 175, 200 microStrain (uStrain) applied the monochromator crystal respectively. Diffracted neutron from the monochromator was monitored by using a neutron camera for evaluating the luminosity and divergence of the beam. The wavelength of the monochromatized beam was calibrated by using a Nickel rod.

1. Introduction

The monochromator is the core component of a neutron diffractometer. The monochromator is used to select the wavelengths of polychromatic neutron beams from the reactor beam tubes. The monochromator is made of a single crystal. The selected wavelengths are those that meet the Bragg equation as follows:

\[ n\lambda = 2d\sin\theta \]

where \( n \) = integer, \( \lambda \) = wavelength (nm), \( d \) = lattice distance (nm), \( \theta \) = diffraction angle

The monochromatized beam is directed to the sample. Then, the lattice distance and any change of it can be measured by means of diffraction method.

Most neutron diffractometers use monochromators with symmetrical diffraction geometry (SDG) configurations. In this configuration, the crystal lattice (hkl) used is parallel to the bulk plane of the crystal. With SDG configuration, the width of the monochromatized neutron beam will be the same as the width of the neutron beam from the source. In the case where the small size of the sample has to be measured, a large amount of the neutron beam is lost and it means that it a relatively small. Or conversely, when a relatively small beam cross-section could be used for measurement of e.g., stylus.

Monochromator with asymmetrical diffraction geometry (ADG) configuration uses a single crystal where the plane (hkl) of the crystal used is not parallel to the main surface of the monochromator crystal slab. With this configuration, you will get different beam widths between those arriving and leaving the monochromator. With this method, it is possible to expand or narrow the width of the resulting beam compared to the width of the source beam. An illustration of symmetrical and asymmetrical geometry is shown in Figure 1.
Applied strain to the perfect crystal will change the perfectness of the alignment of the lattice planes (called as effective mosaicity), and also it has a strong influence on the intensity of the monochromatized neutron beam. The four-point bending system was used for applying the strain to the crystal, as shown in Figure 2.

Four lines bending system will also have a focusing effect on the monochromatized beam in real space. The focal point will depend on the radius of curvature of the crystal and diffraction angle of the beam. The focusing effect will be very clearly seen in the case of SDG.

2. Experiment

The experiment had been performed using a neutron diffractometer for residual stress measurement (DN1). DN1 installed at beam tube #6 of multipurpose reactor GA-Siawabessy located in Serpong, Indonesia. DN1 used single-crystal to monochromatize the neutron beam. The take-off angle of the monochromator manually adjusted from 0 degrees to 90 degrees.

A silicon single crystal (220) slab with a size of 30x200x4 mm$^3$ is placed in the four-line bending system. This crystal has a plane (311) in the direction of 31.5 degrees towards the plane (220). So that the fully asymmetric condition will be obtained by placing the monochromator take-off angle of 63 degrees. The schematic of the crystal position and its placement on the monochromator shielding drum is shown in Figure 4.
The stretching of the crystal is done remotely and controlled by a DN1's computer. The strain occurring in the crystal was monitored using strain-gages also read on the DN1 control computer. The strains applied to the consecutive crystals are as follows: 0, 25, 50, 75, 100, 125, 150, 175, and 200 microStrain.

The monochromatized beam was directed to the sample at a distance of 1500 mm from the monochromator axis. The neutron camera was used to monitor the neutron beam coming from the monochromator. The neutron camera was placed at a distance of 0, 25, 50, 75, 100 cm from the axis of the sample table. The image of the neutron beam captured by the neutron camera was stored electronically. Image processing was performed by using the ImageJ package program, and the width of the beam was calculated by using Origin software. The arrangement of equipment is shown in figure 4.

The monochromatized neutron beam was calibrated by using the Ni-powder. Cadmium mask was used to localized the irradiated area of the nickel sample. Diffracted neutrons were monitored by 2-dimensional neutron detector MWPC and peak position by Origin software.

![Figure 3](image3.jpg)

**Figure 3.** Fully asymmetric diffraction geometry (FADG)

Monochromator in the monochromator drum. The Si(311) planes were 31.5 degrees from the main face parallel to the Si(220). Monochromator take-off angle was 63 degrees.

The stretching of the crystal is done remotely and controlled by a DN1's computer. The strain occurring in the crystal was monitored using strain-gages also read on the DN1 control computer. The strains applied to the consecutive crystals are as follows: 0, 25, 50, 75, 100, 125, 150, 175, and 200 microStrain.

The monochromatized beam was directed to the sample at a distance of 1500 mm from the monochromator axis. The neutron camera was used to monitor the neutron beam coming from the monochromator. The neutron camera was placed at a distance of 0, 25, 50, 75, 100 cm from the axis of the sample table. The image of the neutron beam captured by the neutron camera was stored electronically. Image processing was performed by using the ImageJ package program, and the width of the beam was calculated by using Origin software. The arrangement of equipment is shown in figure 4.

The monochromatized neutron beam was calibrated by using the Ni-powder. Cadmium mask was used to localized the irradiated area of the nickel sample. Diffracted neutrons were monitored by 2-dimensional neutron detector MWPC and peak position by Origin software.

![Figure 4](image4.jpg)

**Figure 4.** Experimental setup with the neutron camera movable along the rail for adjusting appropriate distance 0, 25, 50, 75, 100 cm to the center of the sample table.
3. Results and Discussion
The monochromatized neutron beam image at the sample position (0 cm) at any strain conditions are shown in Table 1.

Table 1. Image of the neutron beam for 0, 25, 50, 75, 100, 125, 150, 175, 200 microStrain applied to the crystal taken at the sample table (0 cm) and the intensity distribution along the line of 0 microStrain of the image.

| Strain (microStrain) | Image | Intensity Distribution |
|----------------------|-------|-----------------------|
| 0                    | ![Image](image1) | ![Intensity Distribution](image2) |
| 25                   | ![Image](image3) | ![Intensity Distribution](image4) |
| 50                   | ![Image](image5) | ![Intensity Distribution](image6) |
| 75                   | ![Image](image7) | ![Intensity Distribution](image8) |
| 100                  | ![Image](image9) | ![Intensity Distribution](image10) |
| 125                  | ![Image](image11) | ![Intensity Distribution](image12) |
| 150                  | ![Image](image13) | ![Intensity Distribution](image14) |
| 175                  | ![Image](image15) | ![Intensity Distribution](image16) |
| 200                  | ![Image](image17) | ![Intensity Distribution](image18) |

The peak intensity distribution at 0, 25, 50, 75, and 100 cm from the sample table as a function of strain applied to the crystal is shown in Figure 5.

Figure 5. Peak intensity as a function of applied strain on the crystal as measured at particular distance from sample table.
Peak intensity distribution as a function of distance to the sample table axis for any applied strain conditions is shown in Fig. 6.

A series of images in Table 1 shows that the strain applied on the crystal also brings about a change of the height of the beam, which looks like a focusing effect.

The peak intensity of the monochromatized neutron beam increases proportionally to the applied strain to the monochromator crystal. This gain was observed at each distance from the sample table. A significant increase occurred in stretching to 75 microStrain. Stretching greater than 150 microStrain does not have much effect on the peak intensity. Stretching greater than 150 microStrain actually causes the distribution of neutron beam intensities to fall apart, as shown in Table 1.

Peak intensity at various measurement positions with respect to the sample table axis shows that the focusing has not occurred at a distance of 100 cm from the axis of the sample table. The peak intensity decreases with increasing the distance from the axis of the sample table is common sense for the neutron beam as a function of distance.

Peak width distributions as a function of distance to the sample table axis for any applied strain conditions are shown in Figure 7.
The peak intensity distribution at 0, 25, 50, 75, and 100 cm from the sample table as a function of strain applied to the crystal is shown in Figure 8.

The peak width of the monochromatized beam was decreased as the stretch increases, as shown in Figure 7. The stretches above 150 microStrain, however, had no big effect on the beamwidth. The slope of the curve in figure 7 is not affected by the applied stretch in the crystal. This shows that the beam divergence is not affected by the applied stretch to the crystal. The average divergence of the monochromatized beam is 7 minutes. This beam divergence is much smaller than the beam divergence of the source file, which is 40 minutes.

Figure 8 shows in more detail the change in the beam width for each stretch condition. In non-stretch conditions, the width of the beam increases by about 6 mm with a change in the distance from the sample table to 100 cm. While at a stretch of 200 microStrain, the beam width only expands by 2 mm.

The diffraction profiles from the Ni powder sample is shown in Figure 9.
Table 2. Calculation results of monochromatic wavelength using Nickel powder as a calibration sample.

| h | k | l | d | 2Theta Meas | Lambda | 2Theta Calc | 1/d Cos Theta | Delta 2Theta |
|---|---|---|---|-------------|--------|-------------|---------------|--------------|
| 1 | 1 | 1 | 2.0344 | 50.21 | 1.7264 | 49.7047 | 0.5428 | 0.5089 |
| 2 | 0 | 0 | 1.7618 | 58.67 | 1.7263 | 58.0641 | 0.6511 | 0.6071 |
| 2 | 2 | 0 | 1.2458 | 87.78 | 1.7273 | 86.6785 | 1.1138 | 1.0999 |
| 3 | 1 | 1 | 1.0624 | 108.70 | 1.7266 | 107.1776 | 1.6149 | 1.5183 |

**Avg=** 1.7266

The peak positions of 2Theta for each diffraction pattern in Figure 9 are fitted by using Gaussian distribution. The peak positions are summarized in Table 2. The wavelength was calculated by using the formula (1). The average wavelength of the monochromatic beam was 1.7266 Angstrom. The offset of the 2theta arm is 0.1662 degrees. The wavelength was matched with Si(311) and the take-off angle at 63 degrees.

4. Conclusion
It can be concluded from this experiment:
A. The applied strain to the crystal with FAGD affected the luminosity of the monochromatized beam and had the minor effect of the focusing in real space.
B. The applied strain to the crystal with FADG has a minor effect on the divergence of the monochromatized neutron beam. The monochromatic beam divergence was smaller than that of the source beam.

C. The wavelength of the monochromatic beam from the FADG monochromator confirms the expectations.

Acknowledgment

The Acknowledgement was conveyed to co-workers at Neutron Scattering Lab. for their cooperation in modifying four line bender to be placed at DN1’s monochromator shielding drum. The acknowledgement is conveyed to co-workers in the reactor division to provide neutrons to conduct this work.

References

[1] Mikula, Pavel & Vrána, Miroslav & Saroun, J & Woo, Wanchuck & Em, V & Čapek, J & Korytar, Dusan. (2016). Comparison of double crystal (+n,-m) and (+n,+m) settings containing a fully asymmetric diffraction geometry of a bent perfect crystal with the output beam expansion. Journal of Physics: Conference Series. 746. 012029. 10.1088/1742-6596/746/1/012029.

[2] P. Mikula, J. Kulda, P. Lukas, M. Vrana, M. Ono and J. Sawano, Instrumentation Components of Focusing Diffraction Used in NPI, ILL, KURRI and PTB, In Proc. of ECNS’99, 1-4 September 1999, Physica B, 276-278 (2000) 174-176.

[3] Rifai Muslih, Ridwan Syarofi, Iman Kuntoro, Nobuaki Minakawa, Applied Stress On Silicon Perfect Single Crystal For Controlling The Extinction Layer, Materials Science Forum 652:255-259, May 2010, DOI: 10.4028/www.scientific.net/MSF.652.255

[4] Mikula, Pavel & Kulda, Jiri & Vrána, Miroslav & Chalupa, B. (1984). A highly efficient double-crystal monochromator for thermal neutrons. Journal of Applied Crystallography - J APPL CRYST. 17. 189-195. 10.1107/S0021889884011274.

[5] J Kulda, V Wagner, P Mikula, J Saroun. Comparative test of neutron monochromators using elastically bent silicon and mosaic crystals. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 338 60-64,1994