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Investigation of Pyrolytic graphite single-crystal (002) plane fine tuning effect on the reflected monochromatic neutron spectra

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HIGHLIGHTS

- Single-crystal graphite grown in highly preferred orientation of (002)-planes known is used in many research centers.
- It can make monochromatic neutron beam the exited neutrons from the radial beam channels of the research reactors.
- It was found that the decrease in reflectivity of the crystal reduces the flux of the monochromatic neutron beam.
- Reducing the mosaic spread of the crystal also reduces the single beam neutron flux.
- The results verified the effectiveness of Vitess and McStas code in modeling the optical components of neutron facilities.

ABSTRACT

Single-crystal graphite grown in highly preferred orientation of (002)-planes known as pyrolytic graphite is used in many research centers to make monochromatic neutron beam the exited neutrons from the radial beam channels of the research reactors. Simulation methods could be effectively used to predict the crystal behavior before time-consuming and high-cost experimental tests. The present work aims to investigate the effect of the PG(002) crystal fine tuning on the reflected neutron spectra quality in Tehran Research Reactor (TRR) D channel neutron beam line. Hence, VITESS3.4 and McStas neutron optic-based computational codes were used in the present work to study the mentioned parameter. To evaluate the obtained code data accuracy a benchmark study was carried out in the present work. The obtained simulations showed that fine adjustment of the crystal angle than the parallel incident neutron beam is very important. In addition, the crystal mosaic spread has noticeably effect on the reflected neutron intensity so that its change from 1.0° to 0.5° decreases the monochromatic neutron peak intensity about 12%. In addition, the simulations showed the crystal reflectivity change from 1 to 0.7 could decrease the monochromatic neutron peak intensity about 43%. Comparison of the experimental monochromatic reflected beam from PG(002) crystal with the carried out simulations showed there is good agreement between the two obtained spectra.

KEYWORDS
PG(002) crystal
Neutron reflection
VITESS3.4
McStas
Computational method

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1 Introduction

1.1 Crystalline neutron monochromator

Today, the use of polycrystalline materials and pyrolytic graphite (PG) has significantly enhanced neutron diffraction techniques. PG has been utilized as a filter for around 30 years. In PG, the crystallites are preferentially aligned along the hexagonal c-axis. When neutrons pass through PG with the c-axis aligned parallel to the beam, the transmission of neutrons shows “absorption” lines resulting from Bragg scattering, depending on the neutron wavelength (Adib, 2009).

It has been demonstrated (Frikkee, 1975) that PG plates can be adjusted for optimal scattering of 2order neutrons across a continuous wavelength range by changing the angle between the c-direction and the incoming neutron beam. If we represent this angle as ψ, and assume that the mosaic spread is minimal compared to ψ, then the lattice planes hkl will scatter neutrons within these specific wavelength intervals:

$$\begin{aligned} &2\,d_{hkl}\sin(\theta_{hkl}-\psi) \le \lambda \le 2\,d_{hkl}\sin(\theta_{hkl}+\psi) \\ &\qquad \text{for} \quad \theta_{hkl} \ge \psi \\ &0 \le \lambda \le 2d_{hkl}\sin(\theta_{hkl}+\psi) \\ &\qquad \text{for} \quad \theta_{hkl} < \psi \end{aligned}$$

Conversely, the filter must be transparent to first-order

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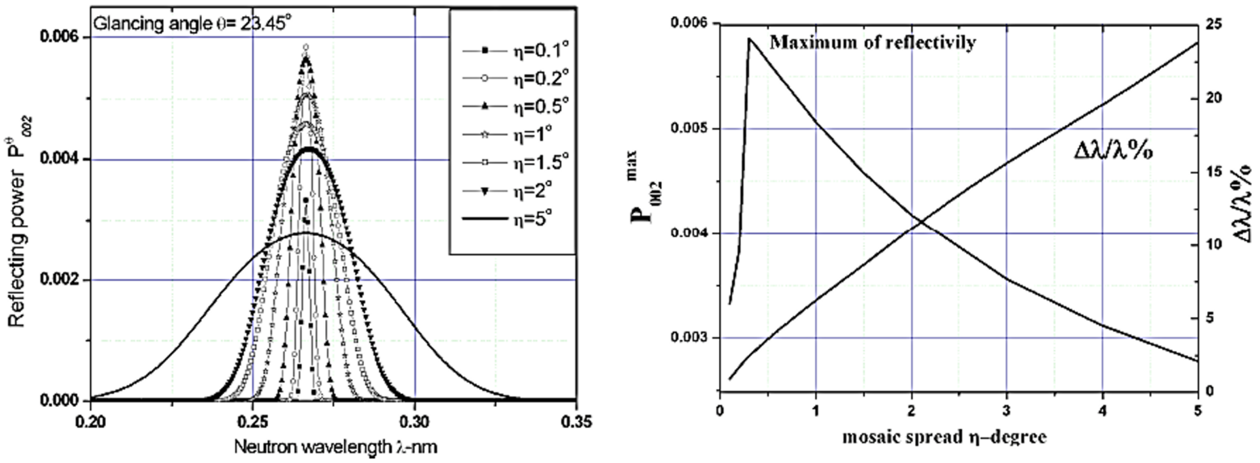

Figure 1: The wavelength distribution of reflectivity from PG at different values of , along with the $\Delta\lambda/\lambda$ (Adib et al., 2011).

neutrons. This range has been identified as covering the wavelength interval of $1.12\ \AA < \lambda/2 < 4.25\ \AA$ [1].

The integrated reflectivity of monochromatic neutrons from PG crystals aligned along their c-axis is significant in the wavelength range of 1 Å to 6.5 Å. The monochromatic properties of the PG crystal are examined in relation to optimal mosaic spread, crystal thickness, and reactor moderating temperature, all of which are important for achieving efficient integrated neutron reflectivity within this wavelength range.

The distribution of reflected neutrons P^{θ}_{002} from PG crystals oriented along the c-axis was calculated by Adib et al (2012). using the following input parameters: PG thickness of 2 mm at a glancing angle of 23.45°, an incident beam divergence FWHM of 0.4°, and a wavelength range from 0.01 Å to 4 Å. The results are presented in Fig. 1. It is observed that a mosaic spread of less than 0.5° yields favorable monochromatic FWHM (Adib et al., 2011).

They theoretically demonstrated that the integrated reflected neutron intensity for the 2nd and 3rd orders from thermal reactor flux can exceed that of the 1st order. This limits the effectiveness of using PG crystals as efficient neutron monochromators, making the use of a neutron filter essential (Adib et al., 2011). In Fig. 2, reflection from a surface is presented.

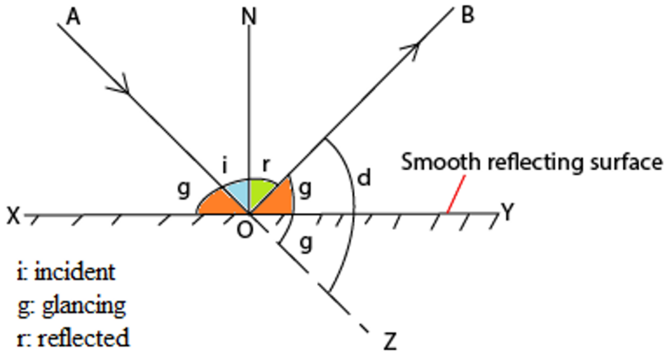

Figure 2: Reflection from a surface.

1.2 Computational neutron-optic codes

The Neutron powder diffractometry facility of Tehran Research Reactor (TRR) was simulated in the reference (Gholamzadeh et al., 2018) using Monte Carlo based programs. The outcomes of the simulation and the experimental data were similar. Theoretical results showed a strong correlation with experimental data, indicating that the VITESS 3.3a code performed well in the neutron optics calculations.

Application of optical codes such as VITESS and McStas (`https://www.mcstas.org/about/`) (Zendler et al., 2014) helps to model behavior optical devices such as monochromator, guide, chopper, crystalline filters, collimator and so on which have been installed in neutron scattering facilities. Many researchers have used the codes to model own facility for calculation of different parameters such as available neutron flux at the sample position, neutron diffraction pattern, transition percentage of neutrons after a crystalline neutron filters and so on. A briefly review on some carried out simulations using the optical codes especially McStas which is more common for such modeling is presented as the following: Paul (2011) used VITESS code to model reflectometer BioRef at Helmholtz-Zentrum Berlin. The carried-out calculations and simulations showed there is potential increase in flux densities, an extension of the momentum transfer range accessible as well as a significant extension of the range of constant wavelength resolution of the instrument (Paul, 2011). Wechsler et al. (2000) VITESS to carry out a comprehensive review of various results calculated with experimental ones. A comparison between powder diffraction based on crystal monochromatization at a CS and a TOF-instrument housed at a LPSS was done using the code. They indicated that VITESS offers the possibility to perform intensity comparisons between different types of instruments considering all three types of sources (Wechsler et al., 2000). Manoshin et al. (2011) indicated VITESS polarized neutron suite allows for the simulation of performance of any existing polarized neutron scattering instrument (Manoshin et al., 2011). Ma et al. (2024) used VITESS code to investigate a conceptual design of a macromolecular diffractometer for the Jlich high brilliance source. They proposed concept for a macro-molecular diffractometer instrument for HBS. The performance of the instrument was evaluated by using VITESS Monte Carlo simulations (Ma et al., 2024).

Alianelli et al. (2004) used a method for detailed simulations of neutron diffraction from imperfect crystals by means of McStas code. Their results showed that the use of Monochromator-reflect allows better simulations of imperfect crystals with McStas (Alianelli et al., 2004). Farhi et al. (2011) used McStas to model experiments in a nutshell: simulating neutron scattering from materials within instruments. They indicated that neutron scattering ray-tracing simulation tools, such as McStas, offer the possibility to model many of these effects, which in the end help to understand the instrument pitfalls and improve their usage (Farhi and Willendrup, 2011). Laliena et al. (2020) used McStas code to model the neutron scattering by a textured polycrystal. They showed that the effect of the texture of the pressure cell on the noise of a diffractogram is very important (Laliena et al., 2020). Tayebfard et al. (2022) used McStas code to model S-shape guides. Their results showed that the guide radius can lead to a cut-off wavelength for neutrons while eliminate fast neutrons and gamma rays (Tayebfard et al., 2022).

Tehran research reactor (TRR) is a pool-type thermal U_3O_8Al plate-type fueled research reactor which its D radial channel has been equipped to neutron diffraction. PG crystal with $2 \times 50 \times 75$ mm^3 dimension is used to make the incident neutron spectrum as monochromatic. The present study aims to investigate the PG crystal fine-tuning effects on the reflected monochromatic neutron beam quality using some optic computational codes. Finally, the obtained results are compared with the experimental results.

2 Research theories

TRR features eight radial beam channels labeled A, B, C, D, E, F, and H (with H being a tangential channel considered as two separate beam channels). Beam channels A, D, E, and H have a diameter of 6 inches and are arranged radially at approximately 30° (see Fig. 3). Beam channels B and F have diameters of 12 inches and 8 inches, respectively, while B arranged radially and F facing directly toward the reactor core (Menarebazari et al., 2023).

VITESS is a widely used software for simulating neutron scattering experiments. Initially developed for instrument design at the European Spallation Source, it now supports all major neutron sources. Researchers can design and optimize both existing and future instruments for reactor or spallation sources, and conduct virtual experiments to prepare for measurements, including basic data evaluation. Reference (Zendler et al., 2014) provides an overview of the VITESS software concept and its applications.

McStas is a versatile tool for simulating neutron scattering instruments and experiment. McStas operates using a compiler that reads a high-level specification language to define the instrument and generates C code for Monte Carlo simulations. It is highly efficient, capable of processing around 500,000 neutron histories per second on a fast PC. McStas supports various configurations, including triple-axis, time-of-flight instruments, and polarized neutrons (`https://www.mcstas.org/about/`) (Potashnikov et al., 2024; Udby et al., 2011). The present work aims to use the mentioned optic codes to investigate TRR PG (002) crystal behavior in front of the parallel neutron beam exited from the first TRR soller collimator.

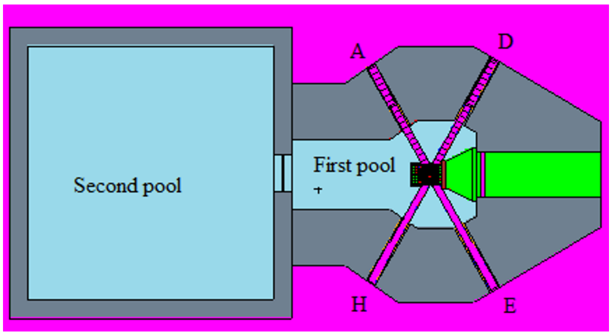

Figure 3: Schematic view of TRR pool and position of its four radial channels (A, D, E, H).

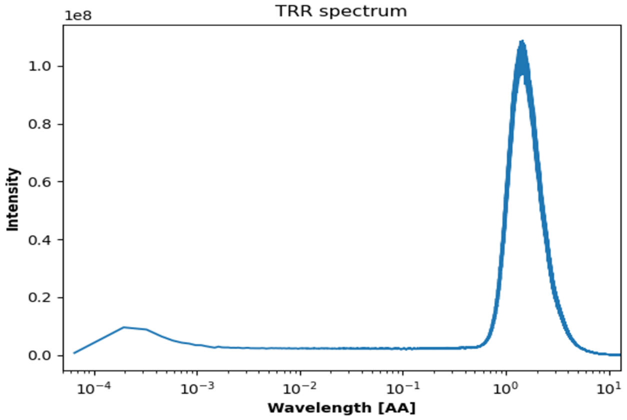

Figure 4: Neutron beam spectrum of TRR in D channel after sapphire crystal.

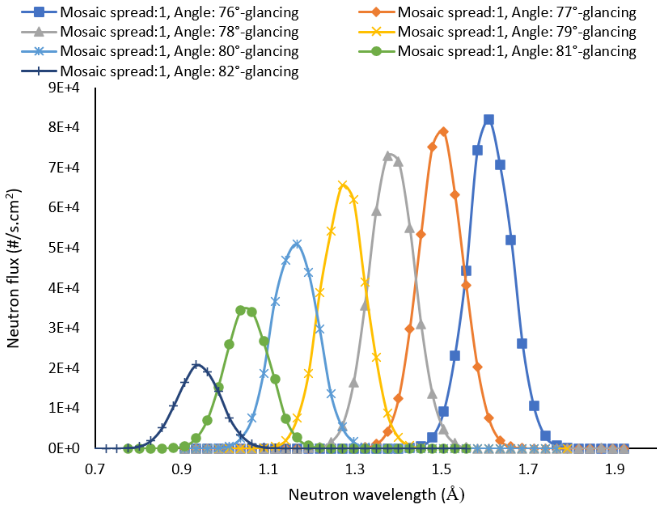

Figure 5: VITESS output for the reflected neutrons from PG(002) crystal with 1° mosaic spread and reflectivity of 1.

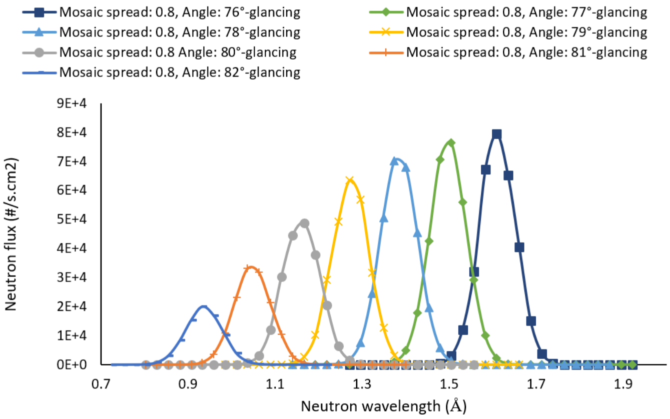

Figure 6: VITESS output for the reflected neutrons from PG(002) crystal with 0.8° mosaic spread and reflectivity of 1.

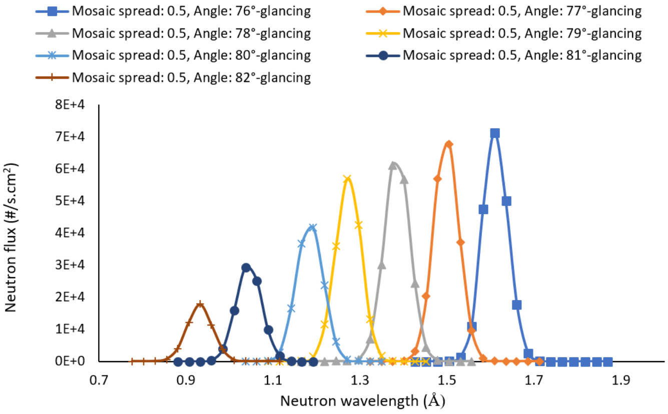

Figure 7: VITESS output for the reflected neutrons from PG(002) crystal with 0.5° mosaic spread and reflectivity of 1.

3 Results and discussion

The spectrum obtained by the MCNP code at the entrance of the D channel of the TRR was used as the input source for the VITESS 3.4 and McStas code. The source is defined as a circular surface source with a radius of 8 cm, in 612 energy groups, and is defined as a “Source gen.” The TRR neutron beam spectrum in the VITESS 3.4 and McStas input files, as a function of wavelength, is presented in Fig. 4.

VITESS code results showed for PG reflectivity of 1 and mosaic spread of 1°, selection of the glancing angle of 13° the angle of the crystal relative to the horizontal plane (77°) would result the highest intensity for the monochromatic reflected beam while the peak for the monochromatic beam is 1.5 $\mathring{A}$. The second highest intensity belongs to the crystal angle of 79° or the glancing angle of 11°, which the peak for the monochromatic beam is 1.3 $\mathring{A}$. The neutron flux peak of the first mentioned monochromatic beam is 24% higher than the second investigated one. In Fig. 5 is shown VITESS output for the reflected neutrons from PG (002) crystal with 1° mosaic spread and reflectivity of 1.

At next stage, the same situation was kept and the crystal mosaic spread was changed to 0.8° in the VITESS input. The same behavior was observed from the Fig. 6 while the neutron flux peak of the 13°-glancing monochromatic beam is 19% higher than the 11°-glancing.

The crystal behavior was investigated for 0.5° mosaic spread as it is depicted in Fig. 7. Again, the neutron flux peak of the 13°-glancing monochromatic beam is 22% higher than the 11°-glancing.

In the D channel, after the sapphire crystal, the first collimator of the diffraction system is located. The collimator is essentially a steel piece with a length of 120 cm, inside which three air channels are embedded. Stainless steel sheets with a thickness of 0.01 cm separate the three air channels from each other and function as a neutron collimator. The window of this collimator has dimensions of 7 × 2.2 cm. After the first collimator, there is a PG (002) monochromator. The length of the second collimator is 60 cm, and the window of this collimator has dimensions of 6 × 2.2 cm. Figure 8 shows the optical equipment installed along the TRR D channel simulated by the McStas code.The behavior of the crystal for 1° mosaic spread was investigated in McStac code at different angles and the results are shown in Fig. 9.

The results of the McStac and VITESS code for the reflected neutrons from the PG(002) crystal with a mosaic spread of 1° and a reflectivity of 1 is shown in Fig. 10.

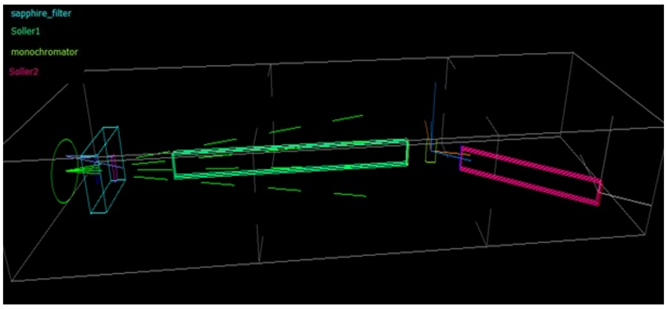

Figure 8: Optical equipment installed along the TRR D channel simulated by the McStas code.

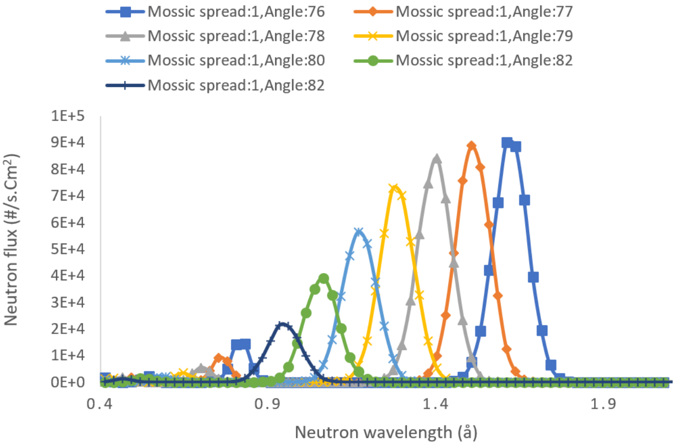

Figure 9: McStac output for the reflected neutrons from PG(002) crystal with 1° mosaic spread and reflectivity of 1.

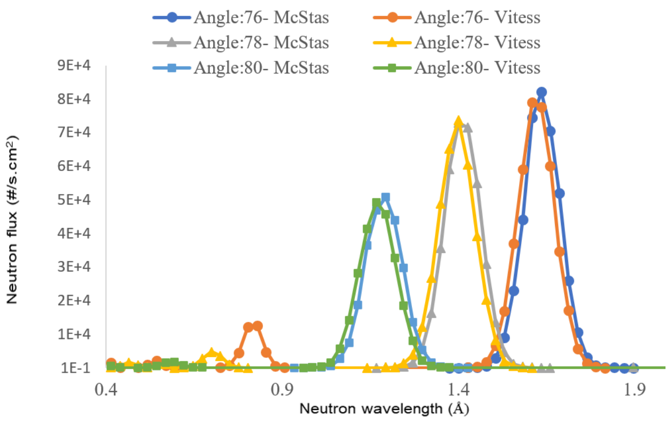

Figure 10: McStac and VITESS output for the reflected neutrons from PG(002) crystal with 1° mosaic spread and reflectivity of 1.

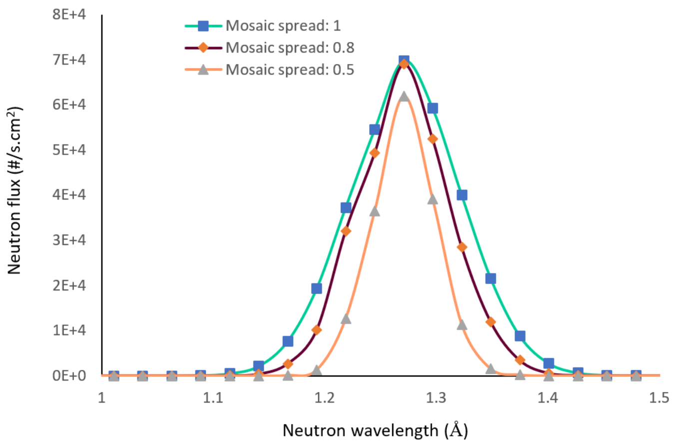

Figure 11: VITESS output for the reflected neutrons from PG(002) crystal with 11° glancing angle and reflectivity of 1.

For crystal reflectivity of 1, the mosaic spread effect on the reflected neutron spectra was compared for glancing angle 11°. The obtained results showed, by mosaic spread reduction the reflected neutron intensity reduces but FWHM of the monochromatic beam improves (Fig. 11). This result is in agreement with the theoretical investigation depicted in Fig. 1. In the case of 0.5 Mosaic spread than 1 there would be about 12% reduction of the monochromatic beam peak.

At the next step, the crystal mosaic spread was selected as 0.5° and the crystal reflectivity was investigated using VITESS code for the crystal glancing angle of 11°. The obtained results showed reduction of the crystal reflectivity from 1 to 0.7 causes about 43% reduction in reflected neutron flux peak (Fig. 12).

A comparison with VITESS 3.4 output and an available PG experimental data was carried out (Fig. 13). As the figure shows there is good comformity between the theoritical calculations and the experimental data of PG(002) in the case of 002 peak position becuse the experimental data has been obtained useing the recorded counts by a detector on n.s^{-1} while VITESS code calculates neutron flux.

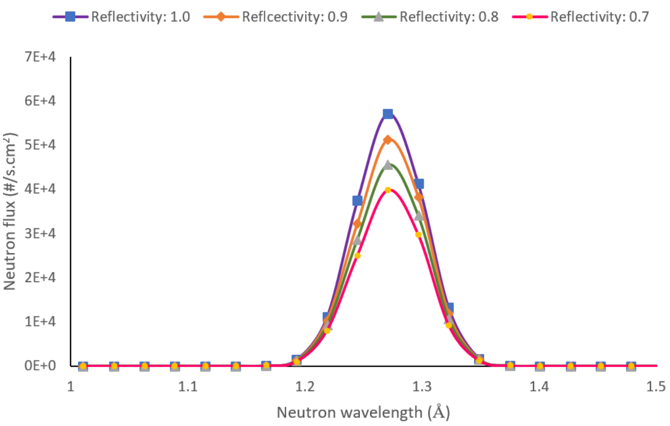

Figure 12: VITESS output for the reflected neutrons from PG(002) crystal with 11° glancing angle and different reflectivity values, Mosaic spread of the crystal: 0.5.

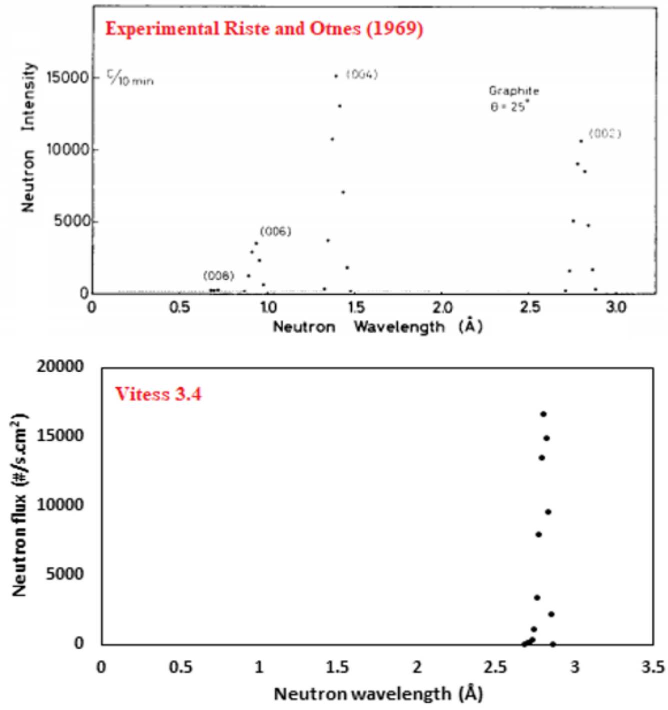

Figure 13: Comparison of VITESS output for the reflected neutrons from PG(002) crystal with 25° glancing angle and the available experimental data for PG crystal (Riste and Otnes, 1969).

4 Conclusions

In the present study, fine tuning effect of single neutron monochromator of PG(002) was investigated. VITESS and McStas code calculations show that the decrease in reflectivity of the crystal reduces the flux of the monochromatic neutron beam. Also, reducing the mosaic spread of the crystal also reduces the monochromatic beam neutron flux. The results obtained by VITESS and McStas code also show their similar behavior regarding the crystal reflection angle changes. Figure 7 also illustrates that the simulation results align closely with the experimental data.

The results of this study can be used to fine tuning of pyrolytic graphite single-crystal (002) plan on the quality of the reflected neutron spectra, including neutron imaging, neutron diffractometry, and neutron scattering facilities. In addition, this work verified the effectiveness of the VITESS and McStas code in modeling and analyzing the optical components of neutron facilities.

Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work.

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