Neutron Optic Simulation For Neutron Diffractometer Facility Of REAKTOR TRIGA PUSPATI (RTP) Using McStas

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ABSTRACT

A neutron diffractometer facility for general purposes is currently developed at the radial beamport of Reaktor TRIGA PUSPATI (RTP). In this paper, a Monte Carlo ray-tracing software, McStas is used to simulate the neutron optic of the facility. The simulations present the optical components which can be manipulated to obtain an optimum component parameters and design of the neutron path for the diffractometer. The performance of the neutron collimation for the facility is presented.

ABSTRAK

Kemudahan neutronometer neutron untuk tujuan umum kini dibangunkan di radial beamport Reaktor TRIGA PUSPATI (RTP). Dalam karya ini, perisian pelacak sinar Monte Carlo, McStas digunakan untuk mensimulasikan optik neutron kemudahan tersebut. Simulasi ini membentangkan komponen optik yang boleh dimanipulasi untuk mendapatkan parameter komponen optimum dan reka bentuk laluan neutron untuk difraksiometer. Prestasi collimation neutron untuk kemudahan dibentangkan.

Keywords: McStas, TRIGA PUSPATI, neutron diffractometer

INTRODUCTION

Neutron diffraction is a non-destructive technique widely used particular for estimating, from the simplest atomic structure to the most complex, structure of crystalline materials [1]. The technique is more powerful than many other characterization techniques such as X-ray diffraction and electron microscopy [2]. Due to the neutron's unique characteristics, neutron diffraction has many advantages over the x-ray technique in terms of contrast, in which the observation of the diffraction pattern effect of light elements in the presence of the heavy ones, the is possible. Furthermore, neutron diffraction has the ability of deep penetration in special conditions or environments as neutrons interact directly with the nucleus of the atom and the strength of neutron scattering differs for different isotopes and magnetic materials [3].

Neutron sources for the neutron diffractometer facilities are provided by nuclear research reactors or accelerators. To select the wavelength of neutron incident on the sample, crystals are usually used as the monochromators. The two types of crystals commonly used as monochromators are bent perfect crystals and mosaic crystals [4]. The resolution in diffraction is based on the monochromator take-off angles, which is the angular dependence of the neutron beam scattered by the sample. In conventional configurations, tight collimation at large monochromator take-off angles are expected to produce good resolutions [5].

Neutron optic simulation is a neutron scattering virtual experiments which models a complete instrument including a sample description. Neutron beams with isotropic intensity distributions and with relatively large wavelength bands produce by the neutron source have to be transported, collimated and monochromated before reaching the sample. The degree of monochromatization and collimation depends on the resolution and intensity needed for the experiment [6]. The neutron optic simulation provides absolute intensity results which can be compared with actual measurements and can be controlled like a real instrument.

Neutron scattering ray-tracing simulation tools, such as Monte Carlo Simulation of Triple Axis Spectrometers (McStas) offer the possibility to model the neutron optic simulation by viewing the effect of the imperfections of existing neutron scattering instruments. This will help in understanding the instrument pitfalls and improve their usage [7]. McStas is usually applied in designing the new neutron scattering instruments, optimizing the flux or resolution of the existing instruments, optimizing the usage of existing instruments for better experiments and possibly compare the virtual with real experiments, during the experiment itself.

MATERIALS AND METHOD

There are several types of neutron diffractometer including single crystal, texture, residual stress, high resolution and high intensity. The type of diffractometer depends on the available reactor power and flux of the reactor. The diffraction technique is well established at the nuclear research reactors with more than 10 MW power and 10^{14} n/cm^2/s neutron flux. For example, the High Flux Isotope Reactor at the Oak Ridge National Laboratory operating at 85 MW with 10^{15} n/cm^2/s neutron flux, hosts 5 diffractometers together with the other 7 diffractometers at the Spallation Neutron Source, which were divided into powder diffraction instruments and single crystal instruments [8]. However, for smaller size facilities, diffraction is quite challenging but possible to be developed with appropriate choice of parameters and components such as established at the Mexican TRIGA MARK III reactor at the Instituto Nacional de Investigaciones Nucleares (ININ) with 1MW power and 10^{13} n/cm^2/s neutron flux [9,10].

Description of RTP

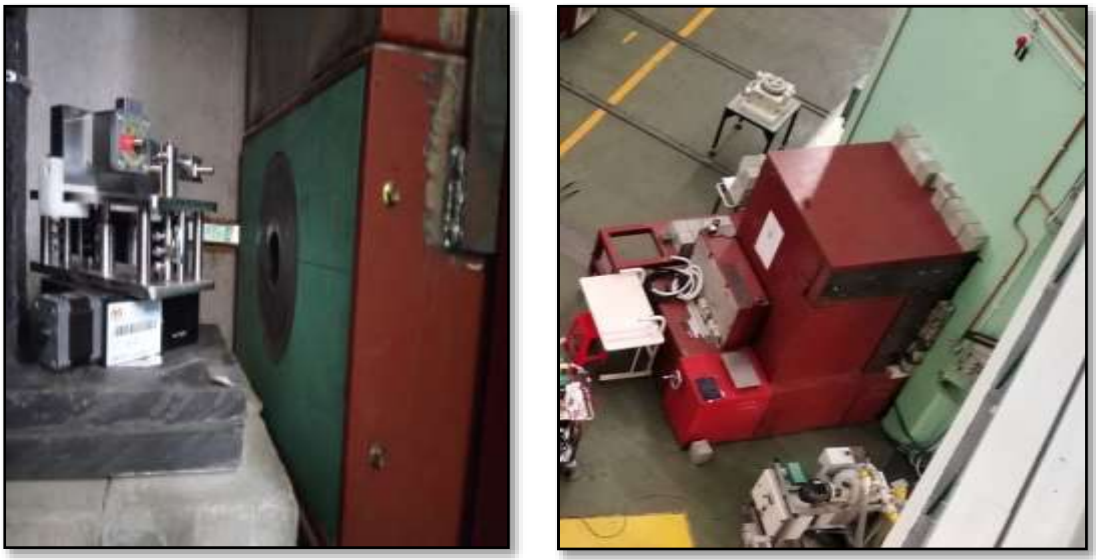
RTP is a 1MW pool-type lightwater TRIGA research reactor. Its fuel assemblies are standard TRIGA $UZrH_{1.6}$ fuel of 8.5, 12 and 20 wt% of U with 19.9% of U-235 enrichment. It has an annular core surrounded by graphite reflector and cooled by natural convection. The reactor is designed to effectively implement the various fields of basic nuclear research including the beam experiments and samples analyses, education and trainings, and production of radioisotopes. It is equipped with irradiation facilities which can be classified into in-core and out-of-core facilities.

The in-core irradiation facilities including the DNA irradiation tube, dry tube, pneumatic transfer system, central thimble, isotope production system, hexagonal irradiation position and triangle irradiation position. The out-of-core facilities are beam ports, thermal column and a rotary rack. There are four beam ports known as BP#1, BP#2, BP#3 and BP#4 which consists of 2 of radial type, 1 of radial piercing type and 1 of tangential type. BP#3 and BP#4 are attached with the neutron radiography (NUR) and small angle neutron scattering (SANS) instrument, respectively. BP#1, BP#2 and thermal column have been considered for neutron diffractometer (ND), prompt gamma neutron activation analysis (PGNAA) and boron neutron capture therapy (BNCT) and these are currently under development.

Neutron Diffraction Facility

BP#1 of RTP is a radial beam port proposed to be used for ND [11]. The value of neutron and gamma ray fluences produced at the end of BP#1 has been determined and the suitable shielding materials has been identified [12]. Images of the ND instrument setting at the RTP are shown in Figure 1. The available ND system consists of collimator, beam shutter, monochromator, beam stopper, sample table and detectors. Illustration of the system setting is shown in Figure 2.

The flexibility in the choice of the monochromator reflections, focus conditions and take-off angles allow selection of instrumental characteristics, which suit the scientific problem, being investigated [13]. In this study, McStas is used to simulate the neutron optic model of ND to determine the reflections of different type of monochromator, focus conditions and take-off angles.



(a) (b)

Figure 1. ND instrument set up at the RTP. (a) monochromator in front of the beam, (b) the shielding system

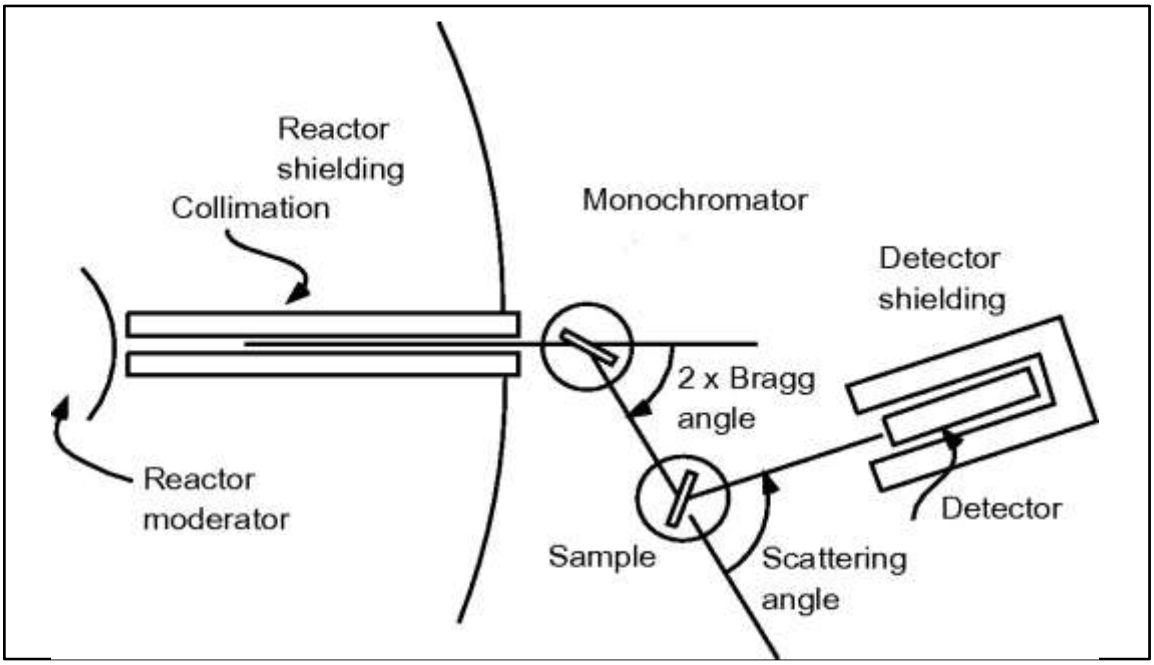


Figure 2. Illustration of ND instrument system at the RTP.

McStas Model

Monte-Carlo calculations have been performed using McStas 2.5 [14]. Simulations were run on a local computer with Windows 10 operating system. The ND instrument was simplified in McStas model that comprised of a reactor moderator acting as the neutron source, collimation slits and guide along the incident neutron path, a monochromator, a beam stopper a sample, a Position Sensitive Detector (PSD) component and virtual monitors "Monitor_nD" and "PSD_monitor" to trace the transmission and reflection of the monochromated neutron. The McStas model as shown in Figure 3 is simulated.

Three type of monochromator Si of single perfect crystal used in this simulation, namely Si(200), Si(311), Si(511).

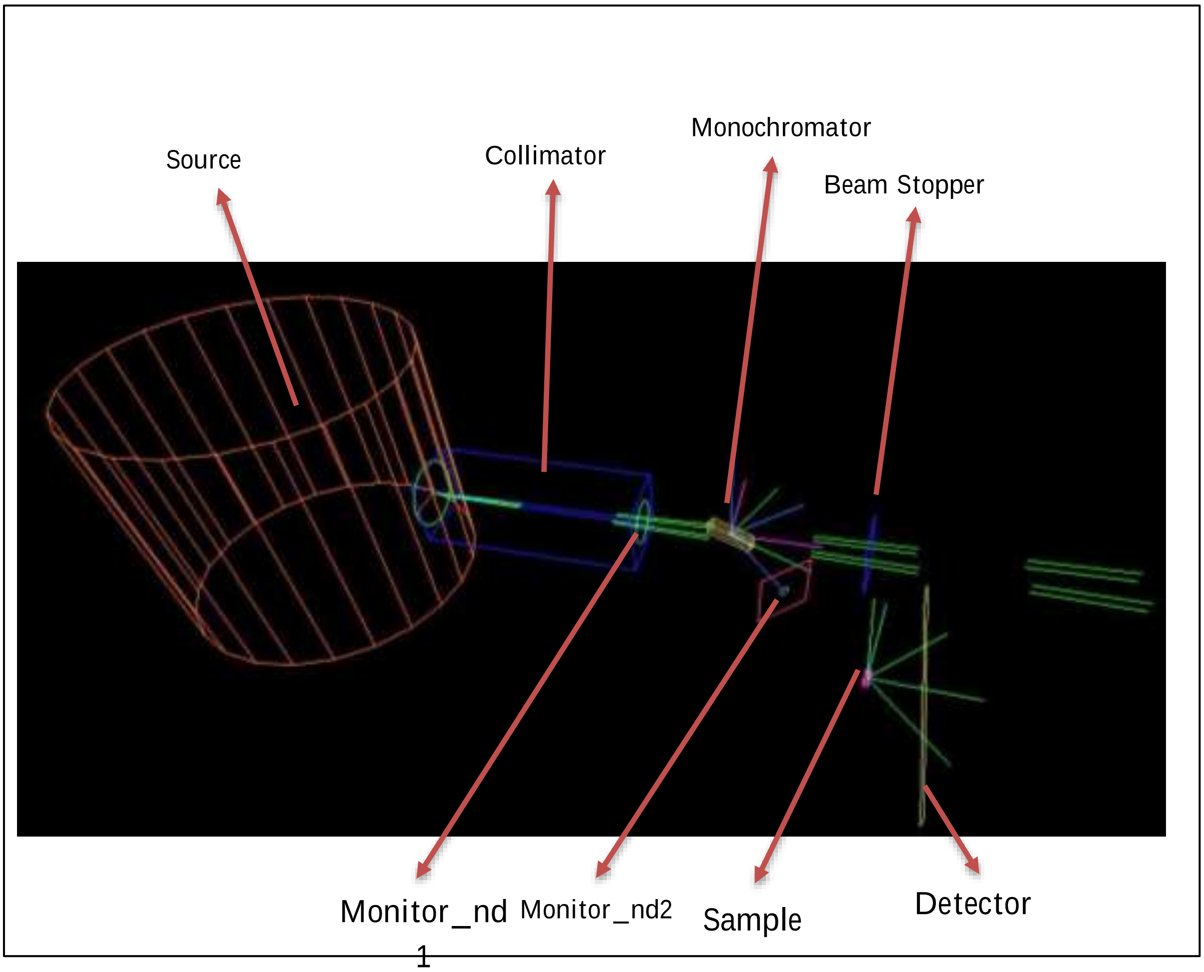


Figure 3. Simplified McStas model of ND at the RTP. Monitor_nd1 is in front of the collimator while Monitor_nd2 is at in front the neutron beam scattered from the monocromator.

Table 1 gives the neutron take-off angle for these monocromators used in the simulation as given by the Bragg's Law:

$$n\lambda = 2d\ Sin\theta \quad (1)$$

where,

n is a positive integer,
λ is the wavelength of the incident wave,
ϑ is the glancing angle where the constructive interference to be at its strongest, and
d is the lattice space of the crystal

Table 1. Neutron take-off angles for Si monocromator			
Monocromator	Lattice spacing d (Å)	Wavelength λ (Å)	Take-off angle x 2 (2θ) deg
Si(220)	1.92	1.53	46.96
Si(400)	1.36	1.5	66.94
Si(511)	1.05	1.5	91.17

RESULTS AND DISCUSSIONS

Figure 4 shows the McStas simulation (top) of the neutron beam intensity versus wavelength and (bottom) the contour of neutron beam after hitting the surface of the monocromator crystal (A) Si(220), (B) Si(511), (C) Si(400) respectively. In this figure, Si(511) shows the highest neutron intensity being scattered as outgoing neutron beam as compared to Si(220) and Si(400).

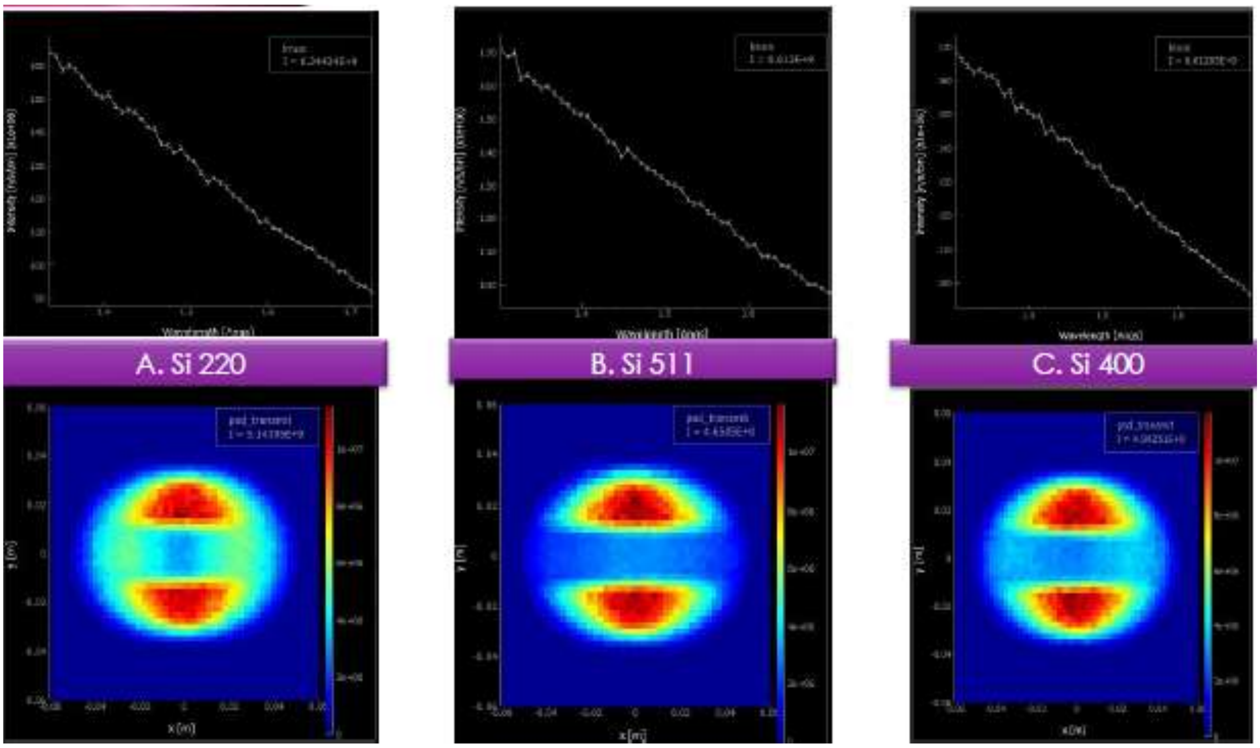


Figure 4. McStas simulation shows (top) the neutron beam intensity versus wavelength, (bottom) the contour of neutron beam after hitting the surface of the monocromator crystal at (A) Si(220), (B) Si(511), (C) Si(400) respectively.

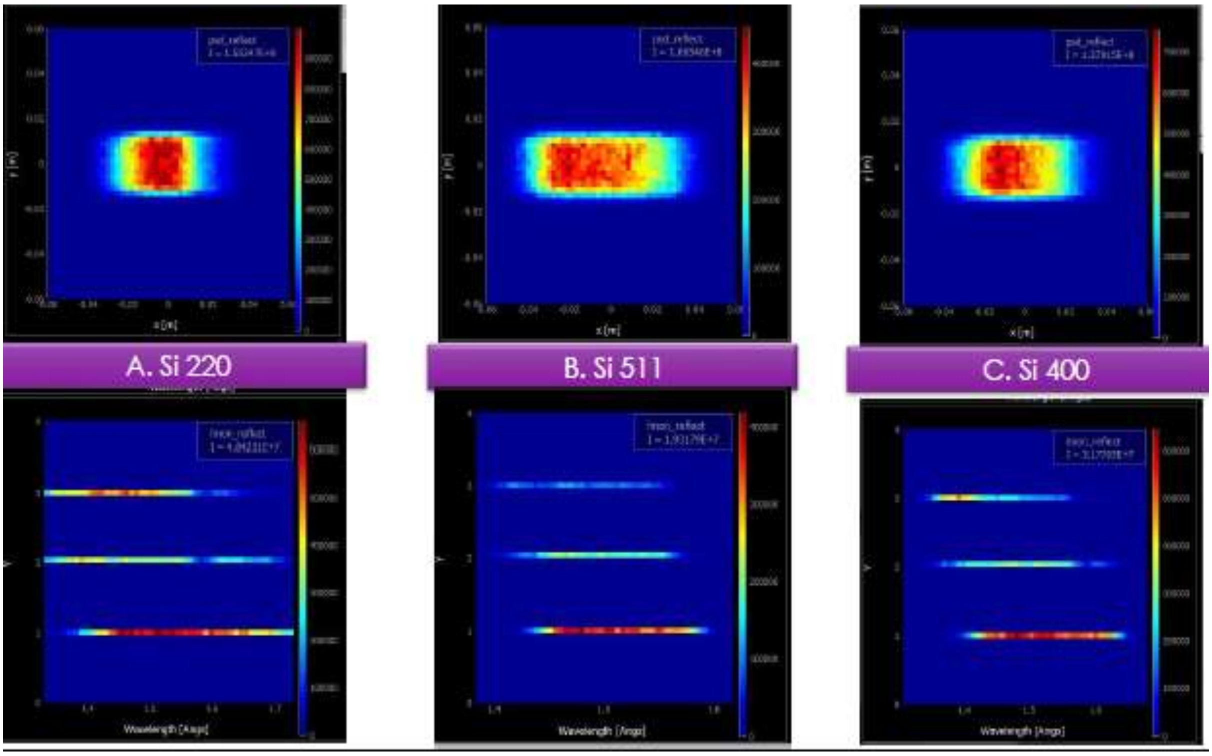


Figure 5. McStas simulation shows (top) the contour of neutron beam from the collimator of beam port#1 hitting the mononcromator surface, (bottom) the contour of neutron beam hitting the three layer of the moncromator crystal (A) Si(220), (B) Si(511), (C) Si(400) respectively.

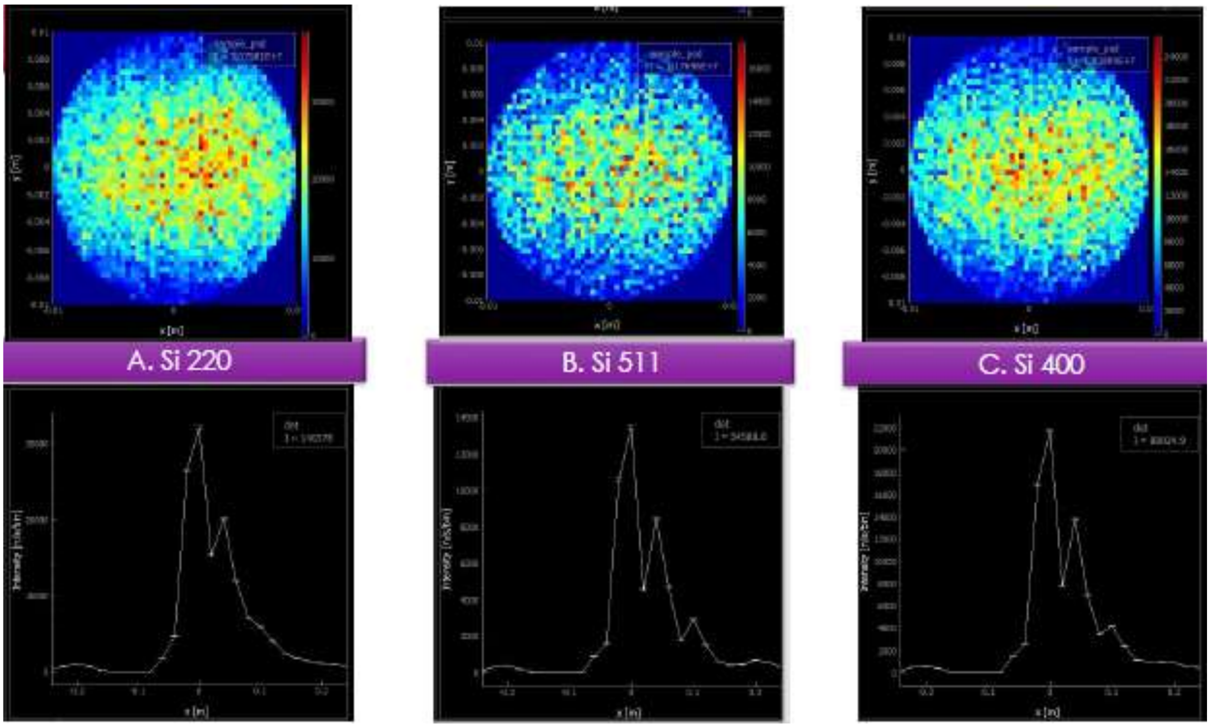


Figure 6. McStas simulation shows (top) the contour of neutron beam from the monocromator port#1 hitting the target sample, (bottom) the plot of neutron intensity versus take angle of diffraction at the sample position using (A) Si(220), (B) Si(511), (C) Si(400) respectively.

Figure 5 shows the instensity neutron beam scattered by monocromator using 3 layers of single perfect crystal of 1mm thick each (at the top) and neutron intensity at each layer of the crystal (at the bottom). Here monocromator Si(511) shows the biggest area of scattered neutrons than Si(220) and Si(400). Figure 6 shows the intensity of neutron scattered at the sample position using monocromator at the top and, at the bottom the neutron couversus diffraction angle at sample position using monocromator (A) Si(220), (B) Si(511), (C) Si(400) respectively.

CONCLUSION

The simulation of McStas has shown that neutron diffraction is feasible at beam port #1 of Reaktor TRIGA PUSPATI (RTP). It also shows that the efficiency of neutron diffraction instrument could be further improved appropriate type of monocromator.

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