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SELECTION OF SUITABLE MONOCHROMATOR & NEUTRON WAVELENGTH FOR TAS AT AERE

M.M. ISLAM[1], M.M. HOSSAIN[2], M.S. ISLAM[3], M.T. ISLAM[4] AND A.A. MAMUN[5]

[1]Assistant Professor, Department of Mathematics and Physics; [2]Assistant Professor, Department of Telecommunication & Electronic Engineering; [3]Lecturer, Department of Electrical & Electronic Engineering; [4]Lecturer, Department of Mathematics and Physics; [5]Assistant Professor, Department of Computer Engineering, Hajee Mohammad Danesh Science and Technology University, Dinajpur-5200, Bangladesh.

Corresponding author & address: M.M. Islam, E-mail: momin_phyhstu@yahoo.com
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ABSTRACT

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Four single crystals Cu(222), Cu(111), Si(111) and PG(002) are used as a monochromator crystal in spectrometer of Atomic Energy Research Establishment (AERE), Savar, Dhaka. The present work consists of a theoretical study in which the suitable range of wavelength of neutron and a monochromator has been chosen for which the diffraction pattern would be contamination free. The neutron flux ratio at half wave wavelength (i.e. percentage of $I_{\lambda/2}$) is determined by examining the Maxwell wavelength distribution of the neutron flux in the TRIGA reactor at AERE. The structure factor ratio of the mentioned monochromator has been calculated. It is found that Neutrons having wavelength 0.05 to 0.95Å are suitable for those monochromators and Si(111) is the best monochromator to get second order contamination free neutron beam for experiments. This may provide a great help in selecting suitable neutron wavelength and proper monochrommator to get 2nd order contamination free patterns.

Key words: *monochromator, Triple Axis Spectrometer (TAS), triga mark-II research reactor*

INTRODUCTION

To perform a neutron scattering experiment, it is essential to have high flux thermal neutron source and a neutron spectrometer (Marshall and Loveasy, 1971). For the neutron source, research reactors are much widely used all over the world. The 3MW TRIGA Mark-II Research Reactor of Atomic Energy Research Establishment, Savar, Dhaka was used for the present experiment.

The TRIGA Mark-II Research Reactor is used mainly for research and isotope production. TRIGA stands for Training Research and Isotope production and GA the suppliers name (General Atomic). There is only one such reactor situated at institute of Nuclear Science and Technology in Atomic Energy in Research Establishment Saver, Dhaka in our country. The TRIGA MARK-II reactor is a light water moderated, graphite reflected designed for continuous operation at a steady state power level of 3 MW and for pulsing with maximum reactivity insertion 1.4% ΔK/K achieving a peak power of about 852 MW. Solid homogeneous mixture of Er-U-ZrH allows containing 19.7wt% U-235, 20 wt % Uranium zirconium hydride and 0.47 wt % Erbium is used as fuel of this reactor. The reactor is located in a reactor tank structure of concrete shield housed in a hall of 20.11×24.4m having a height of 17.35m and is covered by about 6m dematerialized water over the reactor core. An external coolant circuit is used to cool and purify the tank water and this water is circulated at high powers through the core for providing the cooling of the reactor (Hewat 1975). A triple axis spectrometer (TAS) was installed in the radial piercing beam port of the reactor in 1992. TAS can be used for the study of the structural and dynamical properties of crystalline materials. The first axis surrounded by a rotatable massive shielding drum implies a monochromator within which a monochromator crystal is suspended from the top. This is attached to the piercing beam port of the reactor. When the reactor is operated at a power level 3 MW, the beam port contains neutrons of a single wavelength through the process of diffraction and caters to a variety of needs of the experimenter. All the unwanted portions of the reactor beam except monochromator neutron beam coming out through exit port have to be totally absorbed by the shielding arrangement. The shielding in the monochromator drum consists of lead (for gamma-ray), steel (for epithermal neutron partly) boron carbide (for low neutron) and borated paraffin wax for slowing down fast neutron and its subsequent capture (Ahmed *et al.* 1995). Neutron diffraction patterns being the projections of crystal structures in Fourier space carry the information of the sample under investigation. The extent to which the information can be extracted depends largely on the quality of the diffraction pattern. This in turn depends on the proper choice of neutron wavelength and monochromator crystal and also on the proper knowledge of the effect of these parameters for different crystal system. A computer program "FullProf" generally used for the analysis of neutron diffraction data have been utilized for these calculations and generations of neutron diffraction patterns (Juan 1996).

Generally it has been found that the smaller the neutron wavelength, the larger is the intensities. This is because, the interference effect that causes the diffraction of neutron, increases at smaller wavelengths. Thus from the consideration of intensity smaller wavelengths are suitable. However, it has been found that the other factors determining the quality of diffraction pattern gradually worsen with the decrease of λ values. Also the FWHM increases indicating a poorer resolution at small λ values. On the other hand the peaks are well separated with

enhance resolution at higher λ values at the cost of significant loss of intensity and also the reflections at higher with miller indices are missed if the 2θ- scanning range is limited (Rahman *et al.* 2005; Islam *et al.* 2008).

If a crystal used were cut with its surface parallel to (hkl) planes, when oriented to reflect the peak wavelength about λ, it would also be in the correct position to give (2h2k2l) reflection for a half wavelength λ/2. Therefore it is clear that there would be a strong component of this wavelength (second order reflection), giving adulteration of the beam and confusion in interpreting the subsequent diffraction patterns. The condition due to presence of second order reflection in the diffraction pattern produced by half wavelength (λ/2) component in the incident neutron beam is known as second order contamination. But the monochromator beam should not be contaminated by second order. Only less than 1% contamination can be allowed. The contamination may be overcome by using a monochromator reflection where the second order reflection is forbidden. Four single crystals Cu(222), Cu(111), Si(111) and PG(002) are used as a monochromator crystal in spectrometer of AERE, Savar, Dhaka. The aim of our work is to find out the suitable range of neutron wavelength and proper monochromator for which the diffraction pattern would be contamination free.

MATERIALS AND METHOD

When neutrons encounter an atom coherently, they are scattered in all directions isotropically and what we call a diffracted beam is simply a set of scattered beam, which are in phase, so that they reinforce one another. For incoherent scattering this phase relations between the scattered beams are such that they can cancel each other. In the case of neutron scattering from a periodic crystal the condition of coherence, therefore, satisfies just the same as required by the Bragg diffraction that the scattered rays making an angle with the atomic plane equal to the angle of incidence will be in phase with one another. This Bragg law is given as

$$2d \sin\theta = n\lambda$$

Where, n is an integer called the order of reflection and d the spacing of atomic planes in the crystal and θ is the angle between the incident beam and the atomic planes involved. When the neutrons or X-rays encounter an atom, they are scattered in all directions, and what we call a diffracted beam is simply a set of scattered beams, which are in phase, so that they reinforce one another. The Bragg condition is that the rays scattered in the directions making an angle θ with the atomic planes equal to the angle of incidence will be in phase with one another. In all other directions of space the phase relations between the scattered beams are such that they cancel one another. In experimental work, the angle 2θ, rather than θ, is usually measured; it is the angle between the diffracted beam, and the transmitted beam (Cullity 1967).

Scattering from a polycrystalline or powdered sample takes place into Debye-Scherrer cones with the incident $\underline{k}$ direction as axis and semi angle 2θ. Then the total cross-section associated with each cone is

$$\sigma(hkl) = \frac{4\pi^3}{k^2}\frac{N}{V_0}\frac{j}{\sin\theta/\lambda}\left|F_N(\underline{G})\right|^2$$

Where j is the multiplicity of the reflection (hkl). The counter observes only a fraction $\left(l/2\pi r \sin 2\theta\right)$ of the complete cone and,

l = the height of the counter

r = sample to counter distance.

If I is the initial intensity, I is the diffracted beam intensity then

$$I = I_0 \frac{\lambda^3 l}{8\pi r}\frac{VjN_c^2\left|F(\underline{G})\right|}{\sin\theta\sin 2\theta}$$

Where, V is the volume of the sample and N_c is the number of unit cells per unit volume.

For a polycrystalline sample with a vertical circular cylindrical shape, the expression for the experimental intensity can be written as:

$$I = I_0 \frac{\lambda^3 l}{8\pi r}\frac{VjN_c^2\left|F(\underline{G})\right|}{\sin\theta\sin 2\theta}\frac{\rho'}{\rho}A_{hkl}e^{-2\omega}$$

where

ρ' = measured density of the specimen,

ρ = theoretical density,

$e^{-2\omega}$ = Debye temperature correction factor,

A_{hkl} = absorption factor.

Four single crystals Cu(222), Cu(111), Si(111) and PG(002) are used as a monochromator crystal in spectrometer of AERE, Savar, Dhaka (Yunus 1994). The aim of the present work is to find out the suitable range of neutron wavelength and monochromator for which the diffraction pattern would be contamination free. The second order contamination depends upon the following two factors (Bacon 1975).

i. Neutron wavelength spectrum of the reactor,
ii. Strength of (2h2k2l) reflection in comparison to (hkl) reflection from the monochromator.

For a given wavelength spectrum of neutron beam from a reactor, the second order contamination

$$= \frac{I_{\lambda/2} \times F^{(2h2k2l)}}{I_{\lambda} \times F^{(hkl)}} \times 100\%$$
$$= \left(\frac{I_{\lambda/2}}{I_{\lambda}} \times 100\% \right) \times \frac{F^{(2h2k2l)}}{F^{(hkl)}}$$

where,

$I_{\lambda/2}$ = Neutron intensity at the wavelength λ/2 in the spectrum,

I_{λ} = Neutron intensity at wavelength λ in the spectrum.

$F^{(2h2k2l)}$ = Structure factor for (2h2k2l) reflection,

$F^{(hkl)}$ = Structure factor for (hkl) reflection.

In order to investigate the second order contamination at first the neutron flux ratio at half wave wavelength (i.e. percentage of $I_{\lambda/2}$) is determined and secondly the structure factor ratio is calculated. To get the percentage of $I_{\lambda/2}$ for the neutron beam of the TRIGA Mark II reactor, the Maxwell wavelength distribution of the TRIGA reactor given in Figure-1 is examined (Ahmed *et al.* 1995)

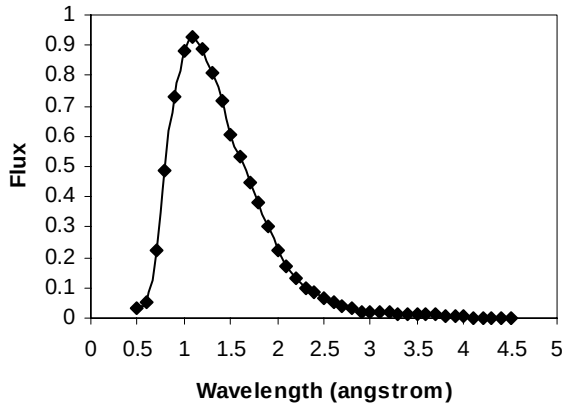

Fig. 1. Maxwell wavelength distribution of the neutron flux in the TRIGA reactor in AERE, Savar, Dhaka.

RESULTS AND DISCUSSION

From the wavelength distribution of the neutron flux the percentage of $I_{\lambda/2}$ for various wavelengths present in the spectrum is calculated and listed in Table-1. Then the Percentage of neutron intensity at the wavelength λ/2 vs neutron wavelength is plotted in fig.2. The reflection strength (structure factor) of principle and second order reflection for Cu(002), Cu(111), Si(111) and PG(002) are calculated and listed in table-2. From this table it is observed that the structure factor of principle and second order reflections are the same order for Cu(002), Cu(111) and PG(002). Whereas the structure factor of second order reflection of Si(111) is zero. Therefore, considering Table-2 the following points can be noted to select the neutron wavelength.

1. Since the structure factor of the principle and second order reflection for the three monchromators Cu(002), Cu(111) and PG(002) are same, therefore, these monochromators will give rise to λ/2 contaminated neutron beam. The strength of the second order reflections from this beam will depend on the strength of λ/2 component in the wavelength spectrum (Fig.1) for the selected wavelength λ. From Table-2 and Fig.2 we see that for this wavelength spectrum 0.5 to 0.95Å of neutrons are free from λ/2

component. So, for these monochromators, the selectable neutron wavelengths should be in the range 0.05 to 0.95Å

2. Since the structure factor of second order reflection of Si(111) is zero the second order contamination of the monochromatic beam is completely forbidden for all neutron wavelength ranges i.e. the hole wavelength spectrum of neutrons (Fig. 5.18) are free from λ/2 component. So any neutron wavelength (higher value) can be used for the Si(111) monochromator crystal to perform experiments.

Table 1. Percentage of neutron intensity $I_{\lambda/2}$

Neutron Wavelength (Å)	**Neutron intensity at the wavelength $\lambda = I_{\lambda}$**	**Neutron intensity at the wavelength $\lambda/2 = I_{\lambda/2}$**	**Percentage of neutron intensity at the wavelength λ/2** $I_{\lambda/2} = \frac{I_{\lambda/2}}{I_{\lambda}} \times 100\%$
3.00	0.018	0.605	3361.11
2.95	0.019	0.623	3278.94
2.90	0.020	0.66	3250.00
2.85	0.028	0.685	2446.42
2.80	0.030	0.72	2400.00
2.75	0.037	0.74	2000.00
2.70	0.040	0.765	1912.50
2.65	0.048	0.79	1645.83
2.60	0.05	0.81	1620.00
2.55	0.058	0.83	1431.034
2.50	0.065	0.85	1307.692
2.45	0.075	0.87	1160.00
2.40	0.085	0.888	1044.70
2.35	0.095	0.9	947.37
2.30	0.100	0.915	915.00
2.25	0.115	0.925	804.34
2.20	0.125	0.93	744.00
2.15	0.15	0.925	616.66
2.10	0.185	0.818	442.162
2.05	0.195	0.89	456.41
2.00	0.255	0.88	345.098
1.95	0.260	0.85	326.92
1.90	0.320	0.81	253.12
1.85	0.34	0.77	226.47
1.80	0.38	0.73	192.10
1.75	0.412	0.67	162.62
1.70	0.45	0.62	137.77
1.65	0.49	0.56	114.28
1.60	0.53	0.43	91.50
1.55	0.563	0.42	74.60
1.50	0.605	0.34	56.198
1.45	0.66	0.265	40.151
1.40	0.715	0.22	30.769
1.35	0.763	0.16	20.969
1.30	0.81	0.12	14.814
1.25	0.85	0.08	9.411
1.20	0.885	0.05	5.649
1.15	0.915	0.04	4.371
1.15	0.915	0.04	4.371
1.10	0.93	0.037	3.978
1.05	0.918	0.033	3.594
1.00	0.88	0.03	3.409
0.95	0.82	0.00	0.00
0.90	0.73	0.00	0.00
0.85	0.62	0.00	0.00
0.80	0.49	0.00	0.00
0.75	0.36	0.00	0.00
0.7	0.225	0.00	0.00
0.65	0.135	0.00	0.00
0.6	0.05	0.00	0.00
0.55	0.04	0.00	0.00
0.50	0.03	0.00	0.00

Table 2. Structure factor for different monochromator

Monochromator	Structure factor of principle reflection	Structure factor of second order reflection
Cu(002)	$4\,b_{Cu}$	$4\,b_{Cu}$
Cu(111)	$4\,b_{Cu}$	$4\,b_{Cu}$
Si(111)	$5.56\,b_{Si}$	0
PG(002)	$16\,b_{PG}$	$16\,b_{PG}$

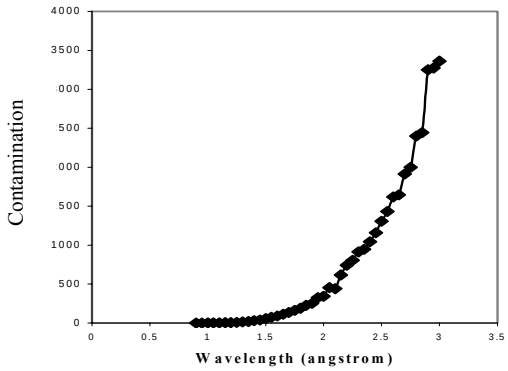

Fig. 2. Second order contamination of the neutron intensity vs wavelength at the **TRIGA** reactor in AERE, Savar, Dhaka.

From the above discussions it is seen that Si(111) monochromator is the best monochromator. Since, neglecting the instrumental limitations of monochromator angle selection a wide range of wavelength can be selected by this crystal without being worried of the second order contamination. However, the choice of monochromator depends on other factors a well. Among them the cost is an important factor. Besides, the reflecting power and mosaicity are also important factors for choosing a monochromator.

CONCLUSION

The structure factors for the Cu(002), Cu(111), Si(111) and PG(002) monochromators crystals available at the triple axis neutron spectrometer at AERE, Savar, have been calculated. From the Maxwell distribution of the neutron wavelengths for the TRIGA Mark II reactor at AERE, each λ and λ/2 component intensity it has been found that the neutrons having wavelength 0.05 to 0.95Å are suitable for the Cu(002), Cu(111 and PG(002) monochromators to get second order contamination free neutron beam for experiments. However, Si(111) monochromator does not reflect any λ/2 component of any neutron wavelength. Thus in this consideration Si(111) has been found to be the best monochromator for AERE spectrometer.

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