Higher-Order Incident Beam Monitor Contamination

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1 Introduction

One of the issues we face when performing triple-axis measurements with fixed final energy involves the nature of Bragg's Law. In satisfying the scattering conditions for neutrons of wavelength λ, we also satisfy the condition for λ/n assuming that reflections with n-times the d-spacing are allowed. Consequently, the beam passing through the incident beam monitor is contaminated by higher order reflections. We typically perform the measurements by counting to a fixed number of monitor counts but this isn't accurate because the amount of higher order contamination is a function of incident energy. In this document, I will try to calculate the fraction of the monitor counts that are due purely to neutrons with wavelength λ. The monitor count should be normalized by this fraction to give a meaningful comparison of intensities at different energy transfers.

The expression for this fraction can easily be written down as:

$$Frac = \frac{Spec(\lambda)R(\lambda)T(\lambda)Eff(\lambda)}{\sum_n Spec(\frac{\lambda}{n})R(\frac{\lambda}{n})T(\frac{\lambda}{n})Eff(\frac{\lambda}{n})} \tag{1}$$

where $Spec$ is the reactor spectrum, R is the monochromator reflectivity, T is the transmission of the upstream Sapphire filter and Eff is the efficiency of the monitor. To accurately calculate the correct fraction, we need valid expressions for each of the terms in the above Equation.

First, we consider the reactor spectrum which is largely defined by a Maxwellian which has a characteristic temperature of about 310K for HFIR. This has the following equivalent forms,

$$\begin{aligned} I(E)dE &\propto E\exp\left[-\frac{E}{k_BT}\right]dE \\ I(v)dv &\propto v^3\exp\left[-\frac{E}{k_BT}\right]dv \\ I(\lambda)d\lambda &\propto \frac{1}{\lambda^5}\exp\left[-\frac{E}{k_BT}\right]d\lambda. \end{aligned} \tag{2}$$

The Maxwellian quite accurately describes the reactor spectrum for smaller energies but the efficiency of the moderation results in an epithermal tail. Sears [1] claims that a reasonable approximation to the reactor spectrum is to assume the Maxwellian for energies up to $5k_BT$ above which

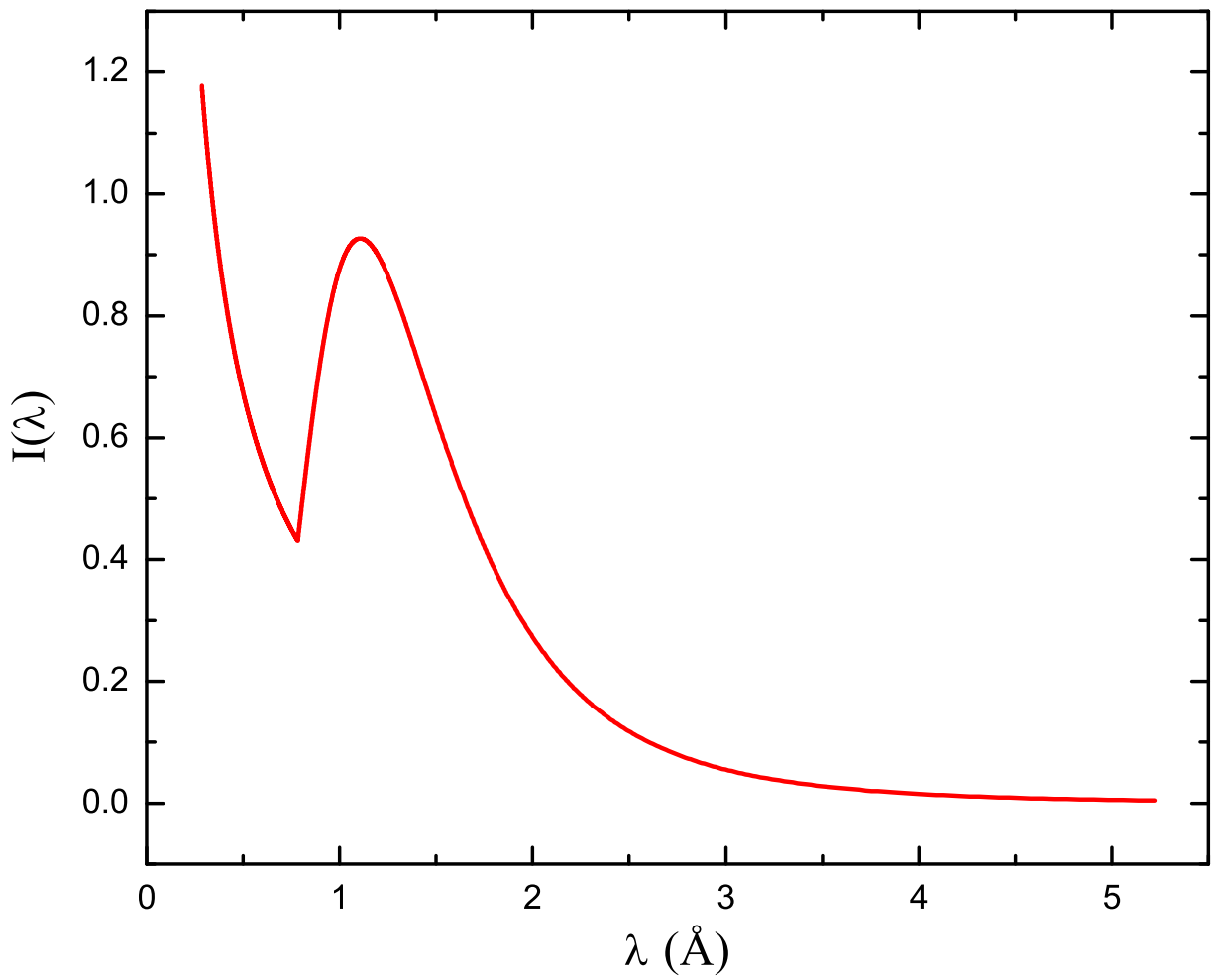

Figure 1: Reactor spectrum including model for epithermal tail as a function of wavelength.

the epithermal tail can be modelled by $I(\lambda) = constant/\lambda$. The resulting plot of $I(\lambda)$ is shown in Figure 1. The cross-over from the Maxwellian to the epithermal tail occurs at λ=$\lambda_0/\sqrt{5}$ where $\lambda_0 = h/(2mk_BT)^{-1/2}$ and the maximum of the Maxwellian is at $\lambda = (2/5)^{1/2}\lambda_0$.

If we write the reactor spectrum as, $f(\lambda)d\lambda$, the appropriate term for higher order wavelengths will be,

$$f(\frac{\lambda}{n})d\frac{\lambda}{n} = \frac{1}{n}f(\frac{\lambda}{n})d\lambda. \tag{3}$$

We must remember to include this factor of 1/n. As a point of interest, if we perform this calculation

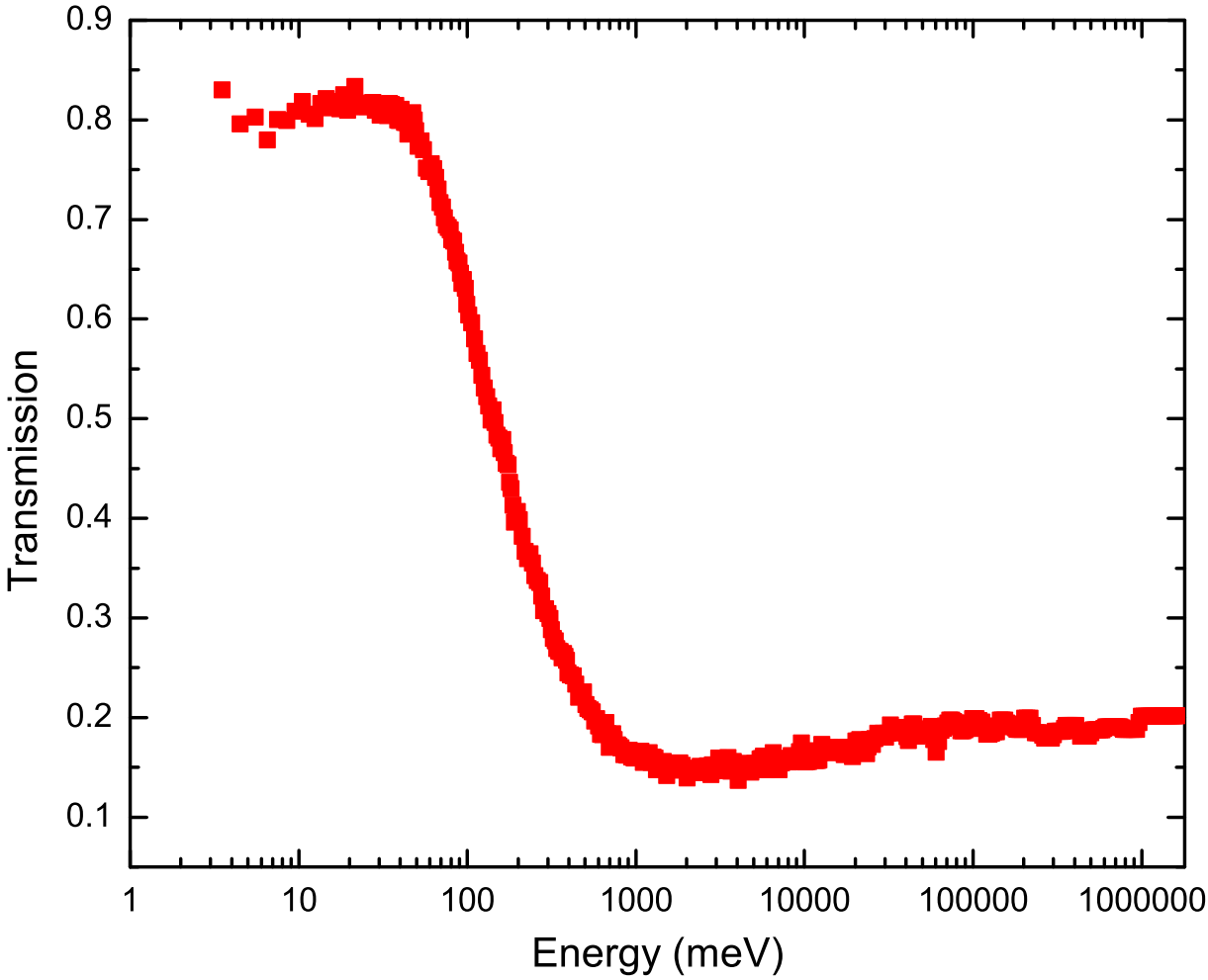

Figure 2: Measured transmission of the Sapphire filter used on HB3 as a function of incident energy.

for the pure Maxwellian, as a function of E, v, and λ, we get

$$\begin{aligned} I(n^2E)dn^2E &\propto n^4E\exp\left[-\frac{E}{k_BT}\right]dE \\ I(nv)dnv &\propto n^4v^3\exp\left[-\frac{E}{k_BT}\right]dv \\ I(\frac{\lambda}{n})d\frac{\lambda}{n} &\propto \frac{n^4}{\lambda^5}\exp\left[-\frac{E}{k_BT}\right]d\lambda. \end{aligned} \tag{4}$$

As a consistency check, we arrive at the same n^4 term for all forms of the Maxwellian indicating a calculation which is independent of how the Maxwellian is formulated.

Single crystal Sapphire has proven to be very useful in thermal neutron scattering experiments as it provides good transmission at small neutron energies and much worse transmission at higher energies. Consequently, it has the net result of greatly suppressing the epithermal tail of the reactor

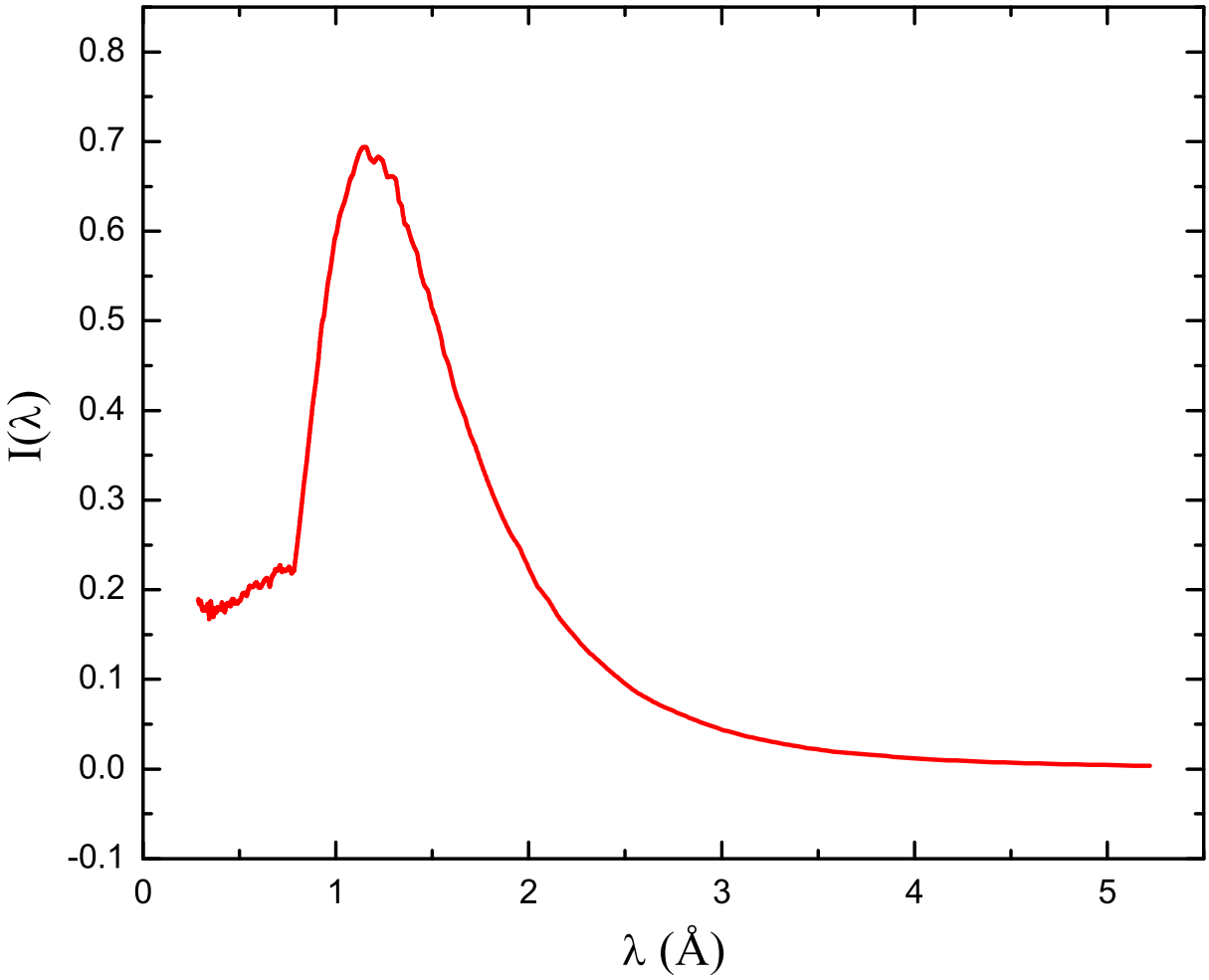

Figure 3: The calculated spectrum shown in Figure 1 multiplied by the Sapphire transmission shown in Figure 2.

ultimately making the spectrum much more Maxwelllian. The transmission of the actual Sapphire filter in place at HB3 was measured at ORELA and the resulting transmission as a funtion of energy (on a logarithmic scale) is shown in Figure 2. To explicitly show the importance of this filter, the transmission shown in Figure 2 has been multiplied by the calculated reactor spectrum (Figure 1) and the resulting curve is plotted in Figure 3. The thermal spectrum is only slightly suppressed by the filter but the epithermal tail of the reactor is greatly reduced.

The calculated reactor spectrum and the measured Sapphire transmission provide three of the four terms needed to calculate the contamination we are interested in. One of the remaining terms is the monitor efficiency which can simply be assumed to be $1/v$. This leaves the final required term, the monochromator reflectivity. This issue is addressed in Sears [1]. For most monochromator crystals, materials are chosen with very small absorption and, consequently, we will ignore the absorption cross-section in this calculation. Sears [1] calculates the reflectivity within the framework of neutron transport theory resulting in reflectivity for the case of a symmetrical reflection (where the incident

Monochromator	PG	Be	Si
Miller Indices	(002)	(002)	(111)
Structure	Hexagonal	Hexagonal	Diamond
Lattice Constants	a=2.4612 Å c=6.7079 Å	a=2.2854 Å c=3.5807 Å	a=5.4309 Å
Unit Cell Volume	$\frac{\sqrt{3}}{2}a^2c$=35.1893 Å^3	$\frac{\sqrt{3}}{2}a^2c$=16.1966 Å^3	a^3=160.1826 Å^3
Scattering Length	6.6460 fm	7.790 fm	4.1419 fm
d-spacing	3.354 Å	1.7904 Å	3.1355 Å

Table 1: Crystal parameters for monochromators used at HB3.

and final angles with respect to the crystal face are the same), R, as,

$$R = \frac{R_k}{1 + R_k} \tag{5}$$

where R_k is the kinematical reflectivity. Within the Gaussian approximation, we can write R_k as,

$$R_k = \frac{1}{\sqrt{2\pi}\eta} Qt \exp\left[-\frac{1}{2}\left(\frac{\theta - \theta_B}{\eta}\right)^2\right] \tag{6}$$

where η is an effective mosaic spread, θ_B is the angle satisfying Bragg's Law for the reflection of interest, t is the thickness the beam sees in the sample (for a symmetric Bragg reflection, this can be written as $d/\sin\theta_B$ where d is the actual thickness of the monochromator). In addition, the crystallographic quantity Q is defined to be,

$$Q = \frac{\lambda^3 |F_B|^2}{V_0^2 \sin 2\theta_B} \tag{7}$$

where V_0 is the volume of a unit cell and F_B is the structure factor for the reflection of interest.

Inserting the expression for R_k (Eq. 6) into the expression for the reflectivity (Eq. 5) results in a maximum reflectivity (occurring at $\theta = \theta_B$) of,

$$R_{max} = \frac{\frac{1}{\sqrt{2\pi}\eta} Qt}{1 + \frac{1}{\sqrt{2\pi}\eta} Qt} \tag{8}$$

with a full-width at half-maximum of,

$$\Delta\theta = \eta \left[8 \ln\left(2 + \frac{1}{\sqrt{2\pi}\eta} Qt\right)\right] \tag{9}$$

The integrated reflectivity, ρ, is defined to be the integral of R over θ and will be proportional to $R_{max}\Delta\theta$,

$$\rho \propto R_{max}\Delta\theta. \tag{10}$$

To calculate the integrated reflectivity, we actually need the detailed crystallographic information for each monochromator crystal of interest. Table 1 shows the relevant crystal parameters for each of the monochromator crystals used at HB3 (PG, Silicon, and Beryllium). The structure factor,

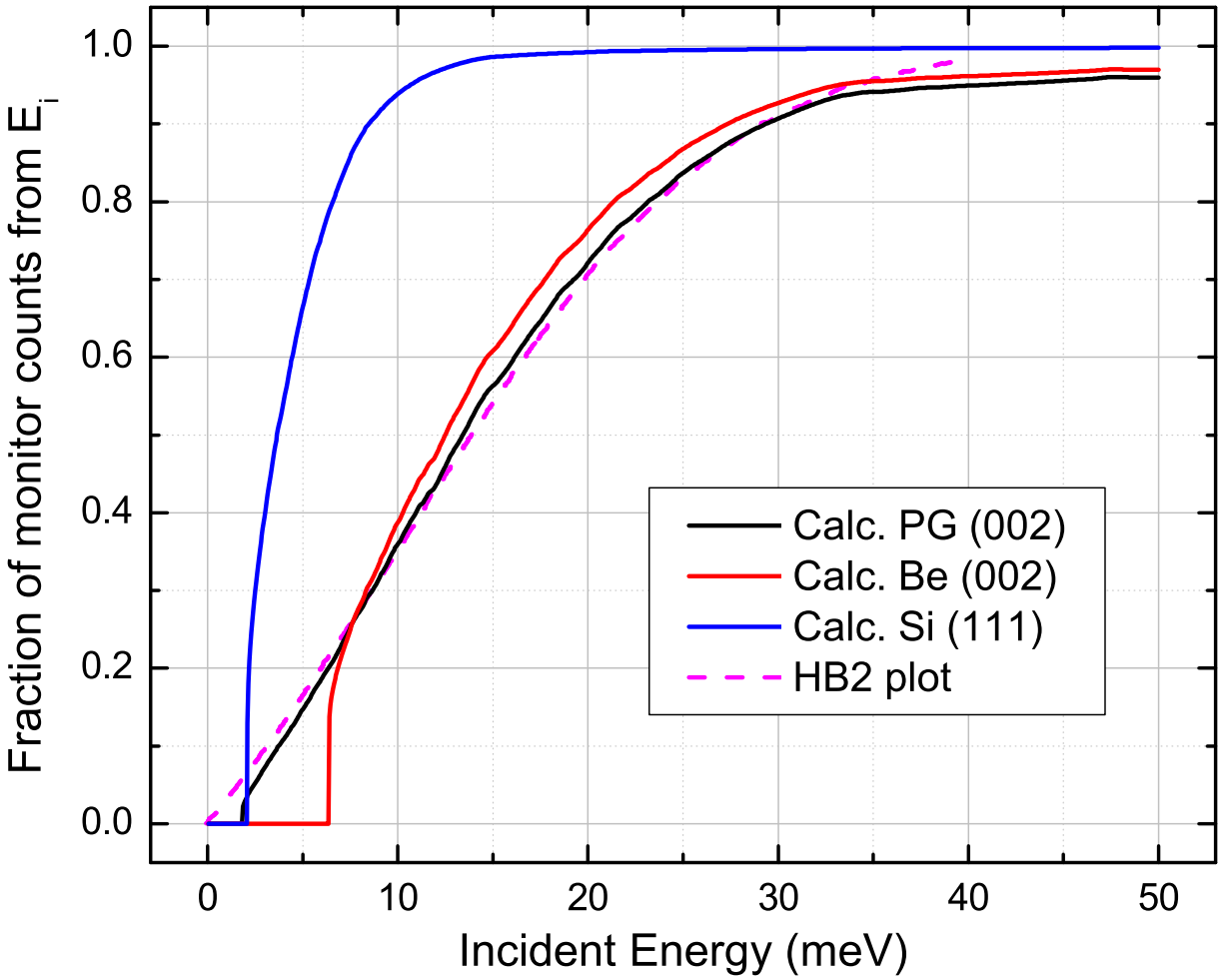

Figure 4: The calculated fraction of monitor counts resulting from E_i for the 3 monochromators used at HB3. For reference, we've included an old plot from HB2 for the PG (002) monochromator used there.

$|F|^2$ for PG along the $(00l)$ direction is zero for l odd and $16b^2$ for those with l even. Note there is a caveat to this - two of the unit cell positions for graphite have a positional parameter z which must be between 0 and 0.05. If set to 0, we get $16b^2$ for all reflections but a non-zero value of z results in a modulation of the structure factor with a periodicity of $1/z$ in l. This causes the structure factor to go to zero at points where l=$1/2z$. For instance, if z has its maximum value of 0.05, the reflection (0,0,10) will have a vanishing structure factor. For the results presented here, we will assume z=0. The simplest structure factor is that of Be for $(00l)$ reflections and is equal to $4b^2$ for l even and 0 for l odd. Silicon has the most complicated structure factor. Reflections along the (hhh) direction with h odd are always present and have an intensity of $32b^2$. Those with h even are present when $3h$=$4n$ where n is an integer and absent when this condition isn't met. The h-even reflections which are present are the most intense reflections with a structure factor of $64b^2$.

We can now calculate the fraction of monitor counts using the expression shown in Equation 1

as a function of E_i and the resulting plot is shown in Figure 4. On this plot, we've included the resulting calculations for PG (002), Si (111), and Be (002). All calculations have been performed numerically using the first 100 orders of reflection. In addition, an old plot from HB2 showing a calculation used there for the PG (002) monochromator. This can be seen to agree very well with the calculation presented here. It differs slightly in both the low energy and high energy regimes. At low energies, a very sharp turn-on is observed and this corresponds to wavelengths longer than $2d$ beyond which Bragg's Law cannot be satisfied for first order reflections resulting in a fraction identically equal to zero. Of course, this turn on is at a very different energy for Be due to the much smaller d-spacing. As all λ/n reflections exist for PG (002) and Be (002), we get very similar curves for these two monochromators. However, Si (111) has several systematically absent peaks (most importantly the $\lambda/2$ (2,2,2) reflection) resulting in a monitor rate which is almost purely due to E_i for energies as low as about 15 meV. Both PG (002) and Be (002) are seen to saturate at a value of about 0.96. This may be due to an overestimate of the fraction of the reactor spectrum included in the epithermal tail. A more reliable functional form for this portion of the spectrum could help here. Such a functional form is difficult to arrive at in the general case as it depends strongly on the detailed moderator configuration in the reactor. For instance, a heavy water moderated reactor with a much larger moderator is much more efficient at moderating the neutrons resulting in a much weaker epithermal tail.

With the code in place to calculate the energy dependent reflectivity for all three monochromator crystals, it is informative to calculate the ratio of the expected neutron intensity from Be and Si to that of PG. According to Sears [1] the expression for the neutron count rate is given by

$$I_{scattered} = \rho\lambda \cot\theta_B I(\lambda) \tag{11}$$

where $I(\lambda)$ is the reactor spectrum as defined above. The ratio can be written as

$$Ratio_{Be,Si} = \frac{\rho_{Be,Si} \cot\theta_{Be,Si}}{\rho_{PG} \cot\theta_{PG}}. \tag{12}$$

The resulting plot is shown in Figure 5. We can see in both cases that the intensity is much smaller than that of PG. For the case of Si, this is due to a much smaller reflectivity (as the d-spacings are very similar between Si and PG). To get better reflectivities from Si, much thicker crystals should have been used but this results in much larger gaps between crystals for the case of a variable focus monochromator. Be, on the other hand, has an integrated reflectivity very similar to that of PG and the smaller intensity is almost entirely due to $\cot\theta$ which is very different due to the different d-spacings. However, for Be, the energy resolution is much improved (due to the same small $\cot\theta$ value) resulting in the traditional tradeoff between intensity and resolution.

References

[1] V.F. Sears, *Neutron Optics,* (New York: Oxford University Press, 1989).

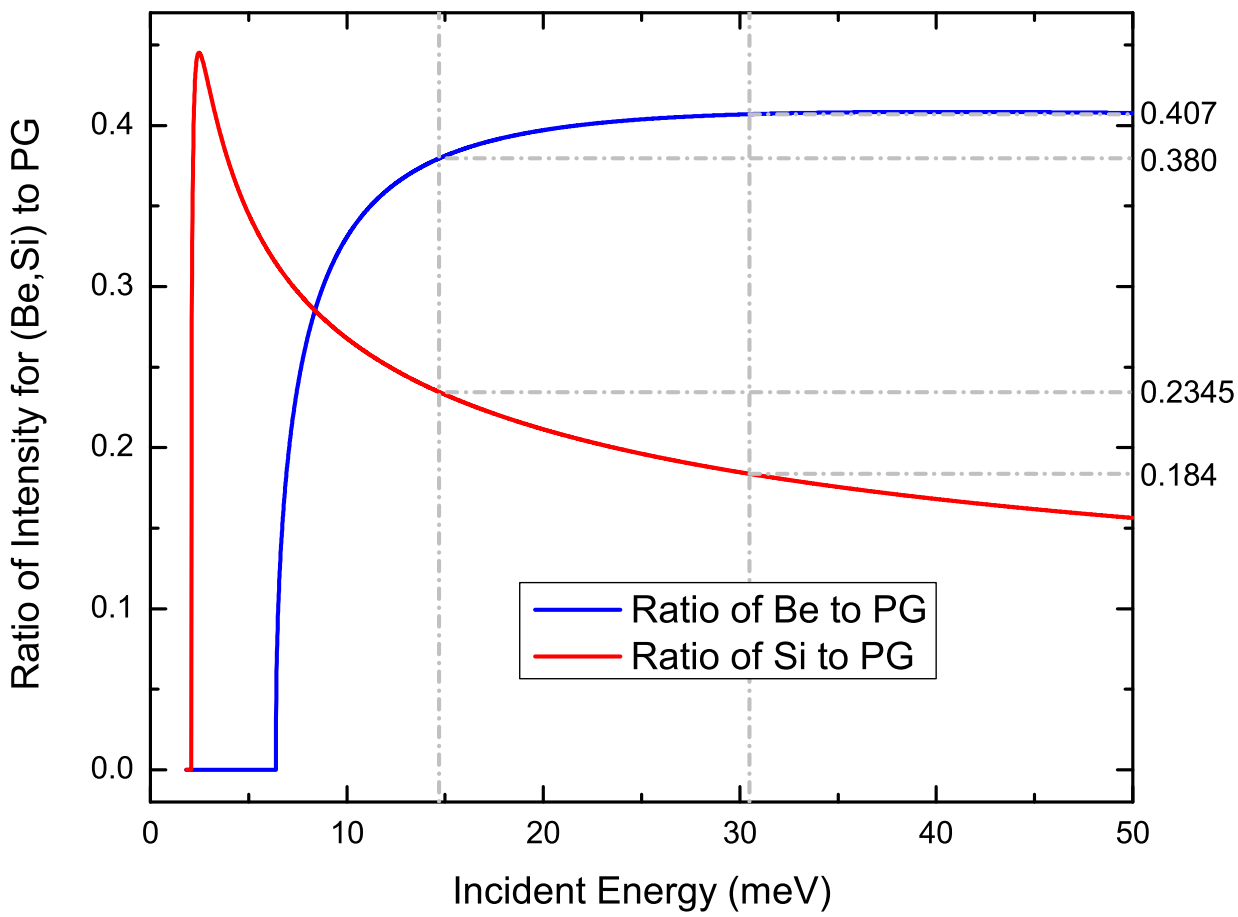

Figure 5: Ratio of the intensity for Be and Si to that of PG. The values for incident energies of 14.7 meV and 30.5 meV are shown on the plot graphically and labelled on the y-axis to the right