A simple formula to calculate the x-ray flux after a double-crystal monochromator

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ABSTRACT

We present a very simple formula for calculating the total number of photons of an x-ray beam after being monochromatized by a double crystal monochromator. This is a typical case for most synchrotron radiation beamlines. The derivation of the formula and its numerical benchmarking by ray-tracing simulations are also presented.

Keywords: Synchrotron, double-crystal monochromator, flux, ray tracing.

1. INTRODUCTION

It is often useful for synchrotron radiation users to estimate the number of photons that impinge on the sample. For that, one has to calculate how the beamline optical elements (filters, windows, attenuators, mirrors and monochromator) affect and modify the spectral flux of the source.

The spectral flux of synchrotron sources is usually given by the number of photons $N(E)$ versus photon energy $E$, per unit of time and per unit of energy bandwidth:

$$\frac{\text{Number of photons}}{\text{sec} \times \text{Energy Bandwidth}}$$

where the energy bandwidth of the source is often given as a value that depends on the energy. It is usually defined as 0.1% of the photon energy:

$$\text{Energy Bandwidth} = \frac{\Delta E}{E} = \frac{\Delta \lambda}{\lambda} = 10^{-3} = 0.1\% \text{ bw}$$

For example, as shown in Fig. 1, the ESRF bending magnet gives about $2.7 \times 10^{13}$ photons/sec/0.1%bw of 8 keV, meaning that the source emits about $2.7 \times 10^{13}$ photons/sec at the photon energy around 8 keV in a bandwidth of $\Delta E = 10^{-3} \times E = 8$ eV, i.e., in the energy interval [7.996, 8.004].

In the case of an optical element that removes photons from the beam, typically an absorber, attenuator, window or filter characterized by a thickness $t$, the flux $N'$ after this element is calculated from the source flux $N$ as:

$$N'(E) = N(E) \, e^{-\mu(E)t}$$

where $\mu(E)$ is the attenuation coefficient, which is energy-dependent. For calculating the number of photons that traverse the element without changing direction nor energy (i.e., those photons that do not interact with the absorber), the attenuator coefficient should include the photoionization, Compton and Rayleigh effects (pair creation energy is

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much larger than the one used in typical synchrotron applications). These terms are tabulated and available in electronic form in a number of computer tools [1-3]. Note that this formula is only valid for photon removal. The energy of the removed photons is fully or partially deposited in the absorber, and other secondary particles (secondary photons and/or electrons) are created in the interaction process. For a detailed simulation of all the processes involved in a typical attenuator, including the spectrum and angular distribution of the exit beam one should use Monte Carlo particle transport algorithms, as implemented in popular particle transport codes (EGS4, PENELOPE, MCNP, GEANT, etc.).

In the case that the beam is reflected by a polished surface (mirror), the flux after the reflection is

$$N'(E) = N(E) R(E)$$

being $R(E)$ the mirror reflectivity obtained from the Fresnel formulas. This reflectivity is dependent on the refraction index; therefore, it depends on the photon energy. It is worth to note the fact that in both formulas (3) and (4) $N'$ is expressed in the same energy bandwidth than the source flux $N$.

![Graph showing flux spectrum](image)

Fig. 1. Dotted line: flux spectrum of the ESRF bending magnet source (for an horizontal divergence of 1 mrad). Dashed line: source spectrum after being transmitted by a beryllium window of 0.5 mm. Continuous line: source spectrum after being transmitted by a beryllium window of 0.5 mm and reflected by a rhodium mirror at grazing angle of 3 mrad.

In this work we address the question of what is the flux after a double crystal monochromator tuned to monochromatize at a given energy. The problem is more complex than those of absorbers and mirrors and, because the monochromator removes photons outside a given energy bandwidth, which is dependent on the selected photon energy (related to the Bragg angle). This problem can be tackled for a particular Bragg angle (or photon energy) using the Du Mond’s diagram, phase space diagrams, reciprocal space diagrams and ray tracing. We present in this paper very simple results that are valid for all Bragg angles. Although these results may appear trivial for many readers, our experience shows that are not so well known for most users and scientists working with synchrotron radiation. Up to our knowledge, no simple formulas are given in literature for answering that question.

2. THE DOUBLE CRYSTAL MONOCHROMATOR

The question of how many photons are available in a synchrotron beam after being monochromatized has been addressed by most beamline scientists and many synchrotron users. We obtained the following formula, which is demonstrated in the appendix:
\[ N_T(E) = N(E) \frac{p_0 \left( \frac{\Delta E}{E} \right)_{\text{intr}}}{\left( \frac{\Delta E}{E} \right)_{\text{src}}} \equiv N(E) R_T \] (5)

where \( N_T(E) \) is the total number of photons after the monochromator (i.e., considering the full energy bandwidth accepted by the monochromator), \( N(E) \) is the number of incident photons in 0.1% energy bandwidth, \( p_0 \) is the peak value of the double-crystal diffraction profile (i.e., the peak of the product of the crystal diffraction profile multiplied by itself, giving \( p_0^2 = 1 \) in first approximation), \( \left( \frac{\Delta E}{E} \right)_{\text{intr}} \) is the intrinsic resolution of the monochromator, equal to \( \omega_D \cot \theta_B \), with \( \omega_D \) the Darwin width of the reflection, \( \theta_B \) the Bragg angle, and \( \left( \frac{\Delta E}{E} \right)_{\text{src}} \) is the energy bandwidth of the incident flux \( N(E) \), in our case a relative energy bandwidth of 0.1% = \( 10^{-3} \).

It should be noted that in some cases, the intrinsic resolution of the crystal is considered constant for a given crystal reflection. Under this assumption, \( R_T \) is a constant with value:

\[ R_T = 1 \times \left( \frac{\Delta E}{E} \right)_{\text{intr}} / 10^{-3} \] (6)

As an example, an x-ray beam with \( N \) phot/sec/0.1%bw, after being diffracted by a double crystal monochromator of Si (111), considering an intrinsic resolution of \( \left( \frac{\Delta E}{E} \right)_{\text{intr}} = 1.35 \times 10^{-4} \) (see next paragraph), we obtain \( R_T = 0.135 \), thus a total number of photons after the monochromator of is \( N_T = N \times 0.135 \). Note that \( N \) is the number of incident photons in 0.1% energy bandwidth and \( N_T \) is the total number of photons at the sample (in the full energy bandwidth transmitted by the monochromator).

Fig 2. The energy dependent intrinsic resolution for a single Si 111 crystal (left) and Si 220 crystal (right). The dependence with energy comes from the structure factor.

3. NUMERICAL VALIDATION

In this section we calculate values of \( R_T \) in several approximations:

- APPROX1) a quick approximation assuming a constant value of the intrinsic resolution in Eq. (6)
- APPROX2) by considering a more accurate (not constant) value of the intrinsic resolution in Eq. (6)
- APPROX3) by doing a numerical evaluation of the double crystal diffraction profile using the results of the dynamical theory of the diffraction, from which we obtain more accurate values of the intrinsic resolution of the crystal and peak value \( p_0 \) and apply Eq. (5)
- APPROX4) by computing \( R_T \) using ray-tracing experiments. We studied a double crystal silicon monochromator at 10, 30 and 50 keV, for (111) and (220) reflections.

The results of this multiple comparison are summarized in Table. 1.
Table 1. Values of $10^4 \times R_T$ for Si crystals at 10, 30 and 50 keV for the reflections (111) and (220) for the different approximations (see text).

<table>
<thead>
<tr>
<th>Crystal</th>
<th>E[keV]</th>
<th>APPROX1 $p_0=1$</th>
<th>APPROX2 $p_0=1$</th>
<th>APPROX3</th>
<th>APPROX4 (RAY-TRACING)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si111</td>
<td>10</td>
<td>1346</td>
<td>1346</td>
<td>1357</td>
<td>1215±36 ($\psi\sim5\omega D$)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1196±29 ($\psi\sim\omega D$)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1206±18 ($\psi\sim\omega D/5$)</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>1325</td>
<td>1337</td>
<td></td>
<td>1367±24 ($\psi\sim5\omega D$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1359±18 ($\psi\sim\omega D$)</td>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td>1356±19 ($\psi\sim\omega D/5$)</td>
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<td></td>
<td>50</td>
<td>1322</td>
<td>1344</td>
<td></td>
<td>1373±30 ($\psi\sim5\omega D$)</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>1362±19 ($\psi\sim\omega D$)</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1362±21 ($\psi\sim\omega D/5$)</td>
</tr>
<tr>
<td>Si220</td>
<td>10</td>
<td>589</td>
<td>589</td>
<td>577</td>
<td>541±13 ($\psi\sim5\omega D$)</td>
</tr>
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<td></td>
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<td></td>
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<td>535±11 ($\psi\sim\omega D$)</td>
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<td>537±11 ($\psi\sim\omega D/5$)</td>
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<tr>
<td></td>
<td>30</td>
<td>572</td>
<td>582</td>
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<td>592±18 ($\psi\sim5\omega D$)</td>
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<td>582±10 ($\psi\sim\omega D$)</td>
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<td></td>
<td>585±10 ($\psi\sim\omega D/5$)</td>
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<tr>
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<td>50</td>
<td>571</td>
<td>587</td>
<td></td>
<td>592±18 ($\psi\sim5\omega D$)</td>
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<td>582±10 ($\psi\sim\omega D$)</td>
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<td></td>
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<td></td>
<td>585±10 ($\psi\sim\omega D/5$)</td>
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</table>

The intrinsic resolution it is usually considered as a constant in first approximation. However, the dependency of the crystal structure factor on photon energy implies that the intrinsic resolution varies slightly versus photon energy. This is illustrated in Fig. 2 for the cases of a single Si (111) and Si (220) crystal reflection.

Let us considered a constant intrinsic resolution value of $\Delta E/E=1.346\times10^{-4}$ and $0.589\times10^{-2}$ for (111) and (220) reflections, respectively, corresponding approximately to the values at energies about 10 keV. Using these values and $p_0=1.0$, we obtain (using APPROX1) $R_T=0.1346$ and $R_T=0.0589$ for Si (111) and Si (220), respectively. It could be also reasonable to choose the asymptotic values for high energies (Fig. 2). However, these values are almost constants for energies greater than about 30 keV and 50 keV for Si (111) and Si(220), respectively, and many synchrotron users work in the lower energy range 5-30 keV. In APPROX1, these values are considered constant for all energies (although it is not strictly true).

For a more accurate result (APPROX2), one must use the intrinsic resolution value from Fig. 2, but we still assume that i) $p_0=1$ and, ii) the intrinsic resolution of the double crystal reflection is the same as a single reflection. The variation of the intrinsic resolution with energy is more pronounced for low energies.

A more accurate approximation (APPROX3) consists in using the dynamical theory of diffraction (e.g., as implemented in the XCRYSTAL application of the XOP code [4]) for calculating the diffraction profile of a single crystal reflection including absorption. Then we compute the diffraction profile of the double crystal reflection, by evaluating product $R\times R$, and we evaluate its peak value $p_0$, and its FWHM (or “improved” Darwin width) that we use to calculate the intrinsic resolution. We use these values in Eq. (5).

In order to benchmark the results obtained with different degrees of approximation and Eq. (5), we have performed ray-tracing simulations using the code SHADOW [5] driven by the SHADOWVUI interface in XOP [4]. We simulated a point source with three different divergences $\psi=5\omega D$, $\psi=\omega D$ and $\psi=\omega D/5$, and then a double-crystal monochromator. The results are shown in the last column of Table 1 (APPROX4). Statistical errors are calculated by averaging ten runs of 25000 rays (per energy) and calculating the standard deviation (1 $\sigma$).
DISCUSSION AND CONCLUSIONS

In this paragraph we discuss the results shown in Table 1 and Fig 3 and extract some conclusions. The ray-tracing calculations give the most accurate results, as it includes for the calculation all the effects presented in the real life and difficult to model analytically (effect source size and divergence, crystal positioning, crystal absorption, etc.). However, the statistical nature produces a different result for each run. We have therefore performed several runs and calculate the average value and standard deviations. The simulations for the three values of the source divergence give the same results within the error bars. This indicates that there is no appreciable difference between the numerical values of the crystal RT value for the sources with different divergences. In a real case, in which the source divergence may be reduced by using a slit, one should consider a RT value independent of the slit size. However, the number of photons N after the slit entering into the monochromator will be obviously reduced by the slit, and this reduction will affect NRT.

From Fig. 3 we see that none of the approximations reproduce the data from ray tracing at lower energies (E=10 keV). However, the value of APPROX3 for Si (111) is not far away from the ray-tracing results. APPROX3 give good results at high energies (30 and 50 keV) and give also the correct curve shape (increasing with energy). APPROX2 (i.e., using the energy dependent value of the intrinsic resolution) give results that are always outside the error bars of the ray-tracing, but the separation from the ray-tracing value is more important for low energies. It is therefore clear, that it is not sufficient to consider the energy-dependent intrinsic resolution of one crystal (APPROX2), but it is important to take into account the intrinsic resolution of the double crystal reflection and use the correct value of p0 (APPROX3).

Regarding APPROX1, it produces a constant value equal to one of the points of APPROX2, value of the intrinsic resolution that is set to a constant. Our choice was to set this constant intrinsic resolution equal to the value at a photon energy equal to 10 keV. This choice has been demonstrated fortunate: the values produced at high energies are closer to the ray-tracing values than those produced using the more accurate APPROX2. An alternative selection of the asymptotic value at high energies would have resulted in much worse results. We should point out that the relative error of the APPROX1 is about 1% for high energies (30 and 50 keV) for both Si111 and Si220 cases, therefore negligible for most applications. For the low energy, the error is about 10%, a value that is acceptable in many cases, especially when trying to make a quick evaluation of the flux during a synchrotron radiation experiment.

These results indicate that, for most applications, it is adequate to use APPROX1 for calculating the flux after a double crystal monochromator. This leads to a very simple recipe:

For estimating the total number of photons transmitted by a double crystal Si (111) monochromator, take the flux spectrum incoming to your monochromator (in the usual units: photons/sec/0.1%bw), and multiply it by 0.135. The
result is, in a very good approximation, the total number of photons versus energy transmitted by the monochromator in the full energy bandwidth accepted by the monochromator (thus, in units phot/sec).

A better approximation (APPROX3) would need the computation of the double crystal diffraction profile and use its FWHM (related to the intrinsic resolution) and maximum ($p_0$). This approximation gives better values or $R_T$, especially at low energies. However, the work involved does not justify the improvement in the values. The most accurate evaluation should be done using full ray tracing.

From these results, it is very easy to include the effect of a monochromator in the spectrum of a synchrotron radiation beam. For example, a Si (111) monochromator placed after a beryllium window and a rhodium mirror, as shown in Fig. 1, would give a flux after the monochromator as shown in Fig. 4 (just multiply by 0.135 and “remove” the “0.1%bw” in the flux label). These calculations can be done very easily using the XPOWER application in XOP [4].

This recipe only applies to flat crystals in the parallel (non-dispersive) configuration. Crystals in antiparallel (dispersive) configuration would give different results. Two crystals curved differently one to another, also present a dispersive affect that would make this recipe not valid. Table 2 presents a list of $R_T$ values for several commonly used crystal reflections. A last comment is that, in theory, a crystal monochromator would be able to monochromatize photons from $\lambda=0$ (corresponding to $\theta_B=0$) to $\lambda=2d$ (for $\theta_B=90$ deg). Obviously, in real monochromators, the mechanical and technical constraints imply that only a smaller range of $\theta_B$ is available, and this implies that the monochromator can only be used in a limited range of photon energy. These constraints have not been considered in our discussion.

![Fig. 4. Dotted line: flux spectrum of the ESRF bending magnet source (for an horizontal divergence of 1 mrad) after being transmitted by a beryllium window of 0.5 mm and reflected by a rhodium mirror at grazing angle of 3 mrad. Continuous line: flux after a double crystal Si (111) monochromator placed downstream from the mirror.](image)

<table>
<thead>
<tr>
<th></th>
<th>Silicon</th>
<th>Germanium</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>(111)</td>
<td>0.135</td>
<td>0.302</td>
<td>0.059</td>
</tr>
<tr>
<td>(220)</td>
<td>0.058</td>
<td>0.136</td>
<td>0.0202</td>
</tr>
<tr>
<td>(333)</td>
<td>0.0087</td>
<td>0.0191</td>
<td>0.0028</td>
</tr>
<tr>
<td>(311)</td>
<td>0.0281</td>
<td>0.0649</td>
<td>0.0091</td>
</tr>
<tr>
<td>(400)</td>
<td>0.0248</td>
<td>0.0564</td>
<td>0.0078</td>
</tr>
</tbody>
</table>
APPENDIX: DERIVATION OF EQUATION (5)

Let us first consider a monochromatic divergent x-ray beam of divergence $\psi$ impinging on the first flat crystal of the monochromator with a Bragg angle $\theta_B$. In this case, the rays that are reflected must impinge onto the crystal with grazing angle $\theta$, in such a way that

$$|\theta - \theta_B| \leq \frac{\omega_D}{2} \quad (7)$$

where $\omega_D$ is the Darwin width of the crystal (the angular range over which total reflection occurs), given by the dynamical theory of diffraction:

$$\omega_D = \frac{2\lambda^2 r_e C}{\pi V} \frac{|F_{hkl}|}{\sin 2\theta_B} \quad (8)$$

being $\lambda$ the photon wavelength, $r_e$ the classical electron radius, $C$ the polarization factor (being 1 for $\sigma$-polarization, usual case for synchrotron monochromators), $\gamma$ the asymmetry ratio (equal to 1 for symmetrical Bragg reflection, considered here), $V$ is the volume of the crystal unit cell, and $F_{hkl}$ is the structure factor for the selected crystal reflection.

The efficiency of the reflection is determined by the geometric ratio $R_1$

$$R_1 = \frac{\omega_D}{\psi} \quad (9)$$

This ratio, valid in the case $\psi \gg \omega_D$, should be modified in the case that both are of the same order of magnitude. In fact, for a collimated beam ($\psi=0$) $R_1$ must be equal to one, because the whole beam is reflected. If we assume that both distributions are approximately Gaussian, they should be added in quadrature, giving then

$$R_1 = \frac{\omega_D}{\sqrt{\psi^2 + \omega_D^2}} \quad (10)$$

Let us consider now the case of a white beam. Every point on the crystal surface reflects photons, but with different energies (wavelengths), depending on the grazing angle $\theta$. Energy and grazing angle must be related by the Bragg equation

$$\lambda = 2d \sin \theta \quad (11)$$

where $d$ is the d-spacing of the crystal. Therefore, we can apply the same argument used for the monochromatic beam when looking at a particular energy that corresponds to the grazing angle $\theta$ (found at a given point on the crystal surface). The beam, after diffraction, will present an energy bandwidth obtained by the derivative of (11)

$$\left(\frac{\Delta \lambda}{\lambda}\right)_{\text{str}} = \left(\frac{\Delta E}{E}\right)_{\text{str}} = \Delta \theta \cot \theta \approx \sqrt{\psi^2 + \omega_D^2} \cot \theta \quad (12)$$
Once again, we have supposed that $\Delta \theta$ is originated from the beam divergence and the Darwin width added in quadrature. If we suppose the beam contains $N$ photons in a bandwidth $(\Delta E/E)_{\text{src}}$, the ratio $R_2$ between the reflected bandwidth and the source bandwidth is

$$R_2 = \frac{(\Delta E/E)_{\text{int}}}{(\Delta E/E)_{\text{src}}}$$  \hspace{1cm} (13)

Therefore, the total number of photons diffracted $N_T$ could be written as

$$N_T [\text{photons/sec}] = N [\text{photons/sec}/(\Delta E/E)_{\text{bandwidth}}] R_T$$  \hspace{1cm} (14)

where $R_T$ is the product of $R_1$ and $R_2$ modified a coefficient $p_0$, the peak value of the rocking curve (i.e., the peak value of the double crystal diffraction profile) to introduce the effect that we are considering two crystals

$$R_T = R_1 R_2 p_0$$  \hspace{1cm} (15)

That can be written as (using (10), (13) and (12))

$$R_T = p_0 \omega_D \cot \theta \left(\frac{E}{E_{\text{src}}}ight)^{-1}$$  \hspace{1cm} (16)

Note that the term $\omega_D \cot \theta$ is the intrinsic resolution of the crystal (Eq. (12) with $\psi = 0$). Therefore, Eq. (16) is identical to Eq. (5). In the case that, in first approximation, the intrinsic resolution is considered independent of the photon energy and Bragg angle, we have:

$$\left(\frac{\Delta \lambda}{\lambda}\right)_{\text{intr}} = \left(\frac{\Delta E}{E}\right)_{\text{intr}} = \omega_D \cot \theta = \frac{4r_d d_{hkl}^2}{\pi V} |F_{hkl}|$$  \hspace{1cm} (17)

Note that the structure factor $F_{hkl}$ is a function of the photon energy through the anomalous scattering factors. The energy-dependent intrinsic resolution of the Si (111) and Si (220) crystals are shown in Fig 2. As the anomalous scattering factors tend to zero at high energies, it is usually said, neglecting this dependence, that the intrinsic resolution is a constant.

**REFERENCES**


