解説

Heat Load Analysis and Resultant X-ray Spectra of a SPring-8 MPW beamline

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The re-emitted spectra and re-emitted power of a hard X-ray traversing solid material have been formulated analytically. The re-emitted X-rays are due to the interaction of the incident X-rays with the material through Compton scattering, Rayleigh scattering and inner-shell vacancy radiative decay. Based on the formula, the re-emitted power of the Compton Scattering, the Rayleigh scattering and the flourescence X-rays are calculated for X-rays from a SPring-8 Multi-pole-Wiggler (MPW) traversing a graphite filter, a Be window and an Al filter. The percentage of the re-emitted power from a Si crystal due to the Compton and the Rayleigh scatterings as a function of the incident angle is also discussed.

1. Introduction

At present time, as well known three so-called third generation synchrotron radiation facilities, European ESRF[1)], American APS[2)] and Japanese SPring-8[3)] are under construction. These machines can produced a tremendous amount of high power X-rays, e.g. of the order of 10 kwatts. The deposition of such X-ray energy brings the problems of heat load in every parts of beamline constituents. The design of beam-line requires many complex calculations of this problem at the cooling system for monochromators, mirrors, absorbers[4-7)] and shielding materials.[8)] Most of these calculations involve X-ray material interaction. In this paper, the re-emitted spectra of the source X-ray traversing a solid material have been formulated analytically. Here the re-emitted X-ray means the X-ray scattered out of the material due to the Compton scattering, the Rayleigh scattering and the X-ray of fluorescence due to the inner-shell vacancy radiative decay. The source X-rays could be any synchrotron radiation beam, white or monochromatic filtered and apertured by an

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arbitrary set of materials or windows. The re-emitted X-rays out of the material can be originated from the source X-rays interaction with the material through Compton scattering, Rayleigh scattering and inner-shell vacancy radiative decay (fluorescence). The detailed physical processes are described as following. (1) The source X-rays are absorbed by the material under consideration through photoionization, the Compton scattering and the Rayleigh scattering. The secondary particles, such as scattered X-rays, photoelectrons are produced. Meanwhile, the inner-shell vacancies are also created by the X-ray material interaction. (2) Some of the secondary X-rays (scattered X-rays, fluorescence X-rays) can be transmitted or back scattered out of the material. (3) The photoelectrons produced by the X-ray material interaction may also escape from the material, but the possibility is so small that it can be neglected.[9] Here, we are only interested in the re-emitted X-rays out of the material and the heat power absorbed by the material. For the convenience of latter discussion, the spectra of the re-emitted X-rays which are originated from the Compton scattering are called the Compton spectra, the spectra of the re-emitted X-rays which are originated from the Rayleigh scattering are called the Rayleigh spectra. The energies of the source X-rays are distributed to either the energy of the transmitted X-rays, re-emitted X-rays and to the heat in solid material. In section 2, theoretical method of the calculation of the Compton spectra and the Rayleigh spectra of transmitted and back scattered is developed. In section 3, the formula are applied to the white X-rays of a SPring-8 MPW traversing a graphite, an Al filter and a Be window. The percentage of the re-emitted power from the Si crystal surface due to the Compton scattering and The Rayleigh scattering as a function of incident angle is also discussed in section 3.

2. Theoretical Method

X-rays lose their energy through the interactions with the material; e.g. the photoionization, the Compton scattering and the Rayleigh scattering. The lost energy is distributed to the kinetic energy of secondary particles, namely, the photoelectrons, the scattered X-rays by the Compton scattering, the Rayleigh scattering and the inner-shell vacancy radiative decay. Among the secondary particles, the X-rays may get out of the specimen either transmitted or back scattered. However the photolectron or the Auger electron is hardly to escape from the material if the material is not very thin. Therefore, the energy of incident X-rays is distributed to the transmitted X-rays, the transmitted, back scattered re-emitted X-rays which come from the Compton scattering, the Rayleigh scattering and the fluorescence processes and heat energy in the specimen.[10] **Figure 1** shows the geometry of the specimen considered and the coordinates system used. Suppose the incident X-ray flux is $F(w)$, the possibility $\eta_a(w, z)$ of the X-ray of energy w absorbed at P position can be written as: (atomic unit $\hbar = m = e = 1$ is used, unless specially mentioned.)

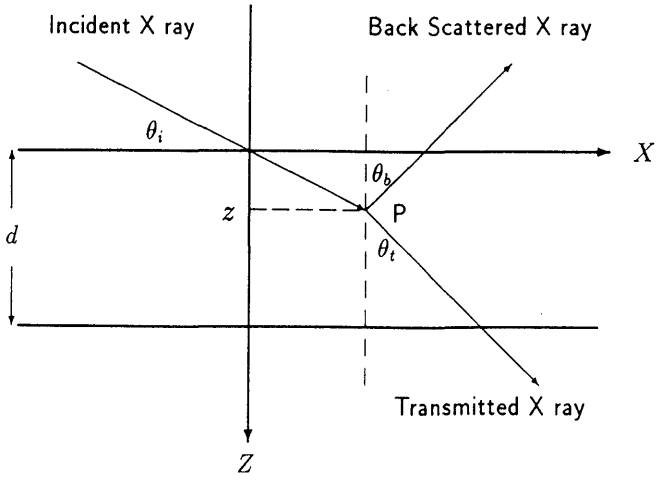

Fig.1 The layout of a specimen and a coordinates system.

$$\eta_a(w,z)\,dz=\mu(w)\bullet e^{-\mu(w)z/\sin\theta_i}\bullet\frac{dz}{\sin\theta_i} \tag{1}$$

where $\mu(w)$ is the X-ray absorption coefficient of the specimen, θ_i the X-ray incident angle with respect to the specimen surface. The possibilities $\eta_t(w',\theta_t,z)$ and $\eta_b(w',\theta_b,z)$ of the X-ray of energy w' at the P position transmitted and back scattered out of the specimen with angle θ_t and θ_b can be written as:

$$\eta_t(w',\theta_t,z)=e^{-\mu(w')(d-z)/\cos\theta_t} \tag{2}$$

$$\eta_b(w',\theta_b,z)=e^{-\mu(w')z/\cos\theta_b} \tag{3}$$

Here, d is the specimen thickness. The re-emitted total powers P_t^c and P_b^c of transmitted or back scattered X-ray out of the material through the Compton scattering can be written as:

$$\begin{aligned}P_t^c&=\int\eta_a(w,z)\,\eta_t(w',\theta_t,z)\bullet\\&\quad F(w)\frac{1}{\sigma_T}\frac{d^2\sigma_c}{d\Omega dw'}\frac{w'}{w}\,dw\,dw'd\Omega\\&=\int e^{-\mu(w)z/\sin\theta_i-\mu(w')(d-z)/\cos\theta_t}\bullet F(w)\frac{\mu(w)}{\sigma_T\sin\theta_i}\\&\quad\frac{d^2\sigma_c}{d\Omega dw'}\frac{w'}{w}\,dwdw'\,d\Omega\,dz\end{aligned} \tag{4}$$

$$\begin{aligned}P_b^c&=\int\eta_a(w,z)\,\eta_b(w',\theta_b,z)\bullet\\&\quad F(w)\frac{1}{\sigma_T}\frac{d^2\sigma_c}{d\Omega dw'}\frac{w'}{w}\,dw\,dw'd\Omega\\&=\int e^{-\mu(w)z/\sin\theta_i-\mu(w')z/\cos\theta_b}\bullet F(w)\frac{\mu(w)}{\sigma_T\sin\theta_i}\\&\quad\frac{d^2\sigma_c}{d\Omega dw'}\frac{w'}{w}\,dw\,dw'\,d\Omega\,dz\end{aligned} \tag{5}$$

Here, the $d^2\sigma_c/d\Omega dw'$ is the differential cross section of the Compton scattering. The re-emitted powers P_t^r, P_b^r, of the transmitted or back scattered X-ray out of the material through the Rayleigh scattering can be written as:

$$\begin{aligned}P_t^r&=\int\eta_a(w,z)\,\eta_t(w,\theta_t,z)\bullet F(w)\frac{1}{\sigma_T}\frac{d\sigma_r}{d\Omega dw}\,dw\,d\Omega\\&=\int e^{-\mu(w)z/\sin\theta_i-\mu(w)(d-z)/\cos\theta_t}\bullet\\&\quad F(w)\frac{\mu(w)}{\sigma_T\sin\theta_i}\frac{d\sigma_r}{d\Omega}\frac{w}{w}\,dw\,d\Omega\,dz\end{aligned} \tag{6}$$

$$\begin{aligned}P_b^r&=\int\eta_a(w,z)\,\eta_b(w,\theta_b,z)\bullet F(w)\frac{1}{\sigma_T}\frac{d\sigma_r}{d\Omega}\,dw\,d\Omega\\&=\int e^{-\mu(w)z/\sin\theta_i-\mu(w)z/\cos\theta_b}\bullet\\&\quad F(w)\frac{\mu(w)}{\sigma_T\sin\theta_i}\frac{d\sigma_r}{d\Omega}\,dw\,d\Omega\,dz\end{aligned} \tag{7}$$

Here, the $d\sigma_r/d\Omega$ is the Rayleigh scattering differential cross section. Similarly, the re-emitted powers P_t^f, P_b^f, due to the X-ray of fluorescence transmitted or back scattered out of the specimen can be written as:

$$\begin{aligned}P_t^f&=\int\eta_a(w,z)\eta_t(w_k,\theta_t,z)\bullet\\&\quad F(w)(1-a_k)\frac{\sigma_k+2.0\ \sigma_c/Z}{4\pi\sigma_T}\frac{w_k}{w}\,dwd\Omega\\&=\int e^{-\mu(w)z/\sin\theta_i-\mu(w_k)(d-z)/\cos\theta_t}\bullet\\&\quad F(w)(1-a_k)\frac{\mu(w)\bullet(\sigma_k+2.0\ \sigma_c/Z)}{4\pi\sigma_T\sin\theta_i}\frac{w_k}{w}\,dwd\Omega dz\end{aligned} \tag{8}$$

$$\begin{aligned}P_b^f&=\int\eta_a(w,z)\eta_b(w_k,\theta_b,z)\bullet\\&\quad F(w)(1-a_k)\frac{\sigma_k+2.0\ \sigma_c/Z}{4\pi\sigma_T}\frac{w_k}{w}\,dwd\Omega\\&=\int e^{-\mu(w)z/\sin\theta_i-\mu(w_k)z/\cos\theta_b}\bullet\\&\quad F(w)(1-a_k)\frac{\mu(w)\bullet(\sigma_k+2.0\ \sigma_c/Z)}{4\pi\sigma_T\sin\theta_i}\frac{w_k}{w}\,dwd\Omega dz\end{aligned} \tag{9}$$

Here, w_k, a_k and Z are K-shell characteristic X-ray energy, Auger yield[11)] and atomic number, respectively. The K-shell vacancies are created through the K-shell photoionization and the Compton scattering processes. The K-shell Compton cross section is supposed to be $2.0 \bullet \sigma_C / Z$, where σ_C is the total Compton scattering cross section. In the same way, we can calculate other inner-shell characteristic X-rays, but it is not important for low Z atom. The X-ray of fluorescence is supposed to be distributed isotopically. The total transmitted X-ray power P_t is obtained as:

$$P_t = \int e^{-\mu(w)d/\sin\theta_i} \bullet F(w)dw \tag{10}$$

Without integration over w' in Eq.4 and Eq.5, the transmitted and back scattered Compton spectra will be obtained. Without integration over ω in Eq.6, Eq.7 and Eq 10, the transmitted and the back scattered Rayleigh spectra transmitted X-ray spectra will be obtained. Based on Eq.4-10, the powers of the transmitted X-ray and the transmitted, back scattered re-emitted X-rays out of the specimen can be calculated. The differential cross section of the Compton scattering involved in the calculation is written as[12,13]:

$$\frac{d^2\sigma_C}{d\Omega dw'} = \frac{Z \bullet r_0^2}{4}\left(\frac{w'}{w}\right)^2 \sum \left[\left(\frac{w'}{w}\right) + \left(\frac{w}{w'}\right) - 2.0 + 4\vec{e}_1\vec{e}_2\right]$$

$$\delta\left(w' - \frac{w}{1 + \frac{w}{mc^2}(1-\cos\theta)}\right). \tag{11}$$

The polarization vectors of the incident and scattered X-ray are denoted by $\vec{e}_1$ and $\vec{e}_2$. Under the form factor approximation, the Rayleigh scattering cross section is written as[14,15]:

$$\frac{d\sigma_R}{d\Omega} = \frac{r_0^2}{2} f^2(q)(1 + \cos^2\theta). \tag{12}$$

Here

$$f(q) = \int \rho(r)\frac{\sin qr}{qr} 4\pi r^2 dr \tag{13}$$

is so called atomic form factor and $q = \sqrt{2k^2(1-\cos\theta)}$ is the magnitude of momentum transfer. $\rho(r)$ is atomic electron density which can be written as[16-18]:

$$\rho(r) = \frac{Z}{4\pi r}\left[A\alpha_1^2 e^{-\alpha_1 r} + (1-A)\alpha_2^2 e^{-\alpha_2 r}\right], \tag{14}$$

where A, α_1, α_2 are parameters which have been listed for some atoms and solid materials[15,16]. Therefor the form factor can be easily obtained after simple calculation.

$$f(q) = Z \bullet \left(\frac{A\alpha_1^2}{\alpha_1^2 + q^2} + \frac{(1-A)\alpha_2^2}{\alpha_2^2 + q^2}\right). \tag{15}$$

The absorption coefficient $\mu(w)$ of the specimen is also calculated as discussed in the previous paper.[19] Generally speaking, the X-ray beam divergence is less than 1 mrad for the SPring-8, much smaller compared with the incident angle θ_i. So, we assume that the θ_i is the same for all the incident X-rays.

In the formula, the re-emittion of the third X-rays due to the interaction of secondary X-rays with the specimen is not taken into account because the power re-emitted due to the third X-rays is very small compared to the power re-emitted by the secondary X-rays. If the specimen thickness d is much larger than the electron stopping length which is of the order of μm (this condition is satisfies almost in all case), few photoelectrons can escape from the specimen. Thus, the total incident power can be divided into three part, i.e, the transmitted power, the re-emitted power out of the specimen and the heat power of the specimen. Using these calculated data, one can design various optical devices such as a filter, a mirror and a monochromator. In the next section, the re-emitted power of the X-rays of the SPring-8 MPW beam line traversing a graphite, an Al filters and a Be window will be discussed based on Eq.4-10.

3. Application to a SPring-8 beamline

Figure 2 shows a schematic figure of typical beamline setup as will be used in the SPring-8 beamlines. The X-rays generated from insertion device MPW (multipole wiggler) will go through a graphite, an Al filter and a Be window and inject on a Si crystal monochromator into an experimental chamber. The reason we use the graphite filter as the first optical element is that graphite can stand for a huge heat power. The Al filter is used to absorb low energy X-rays which are not interesting to beam users. The Be window is used to separate the UHV chamber from the user's experimental chamber. Here, we will first discuss the characteristic of the beamline. Then, we will discuss the set of the filters; the combination of graphite, Al and Be windows.

A. The SPring-8 MPW beamline

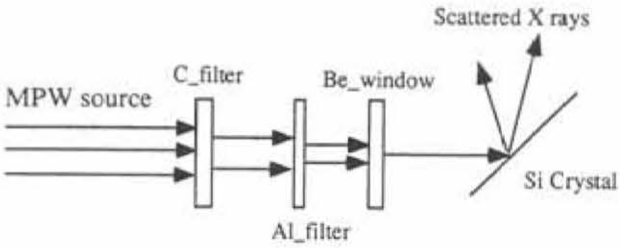

Fig.2 An optical elements alignments of the SPring-8 MPW beamline.

Table 1 The beamline parameters of the SPring-8 MPW.

E (GeV)	8.0	I (mA)	100
σ'_x (mm)	0.082	σ'_y (mm)	0.074
σ_x (mrad)	0.076	σ_y (mrad)	0.009
K	16	ω_1 (keV)	0.026
λ_c (cm)	18	L (m)	3.96
ω_c (keV)	40.5	P (kW)	14.54
σ^R_x (mrad)	0.64	σ^R_y (mrad)	0.037

The electron beam in a storage ring is characterized by the electron beam energy E, beam current I, beam spatial and angular divergences ($\sigma_x, \sigma_y, \sigma'_x, \sigma'_y$). The synchrotron radiation from an insertion device (MPW or undulator) is characterized by K parameter, periodic length λ_c, total length L and the fundamental energy of the first harmonic oscillator w_1, the critical energy w_c, the total output power P, the power angular divergences (σ^R_x, σ^R_y). The relative parameters of the SPring-8 MPW is shown in **Table 1**. The total output power 14.5 kW is the heat source for all optical elements. While such a huge power is concentrated in a very small angle as shown in **Fig.3**. The divergence on the vertical direction is much smaller than that on the horizontal direction due to the large K. Here we consider that the electron beam divergence is zero. The real X-ray divergence is larger than what is shown in **Fig.3** because of the electron beam divergence. But, we can see that the electron beam divergence is smaller than the divergence of radiated X-ray; the electron beam divergence dose not strongly influence the radiation divergence in this case.

B. Heat power distribution of the C-Al-Be filters set

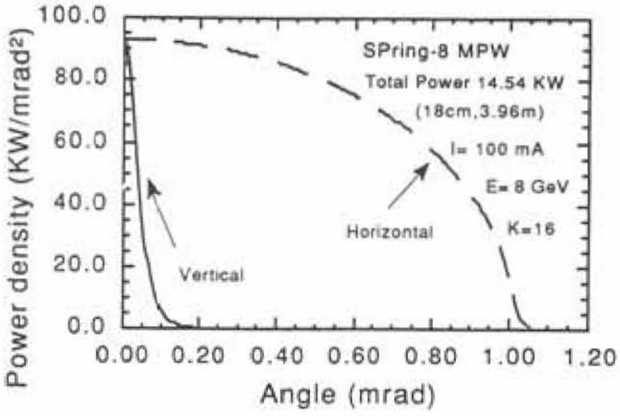

Fig.3 Power angular density of the SPring-8 MPW beamline.

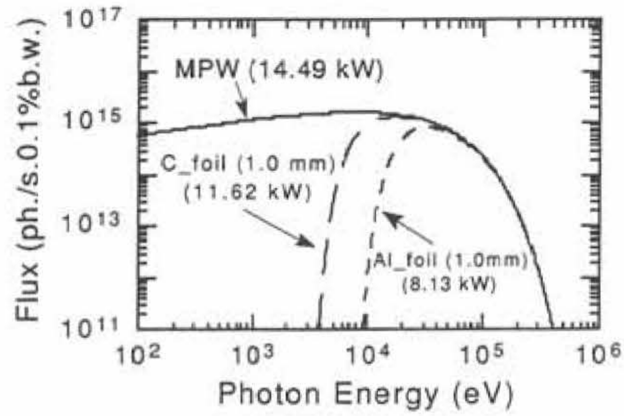

Fig.4 X ray fluxes of the MPW, flux after the graphite filter and flux after the Al filter, respectively.

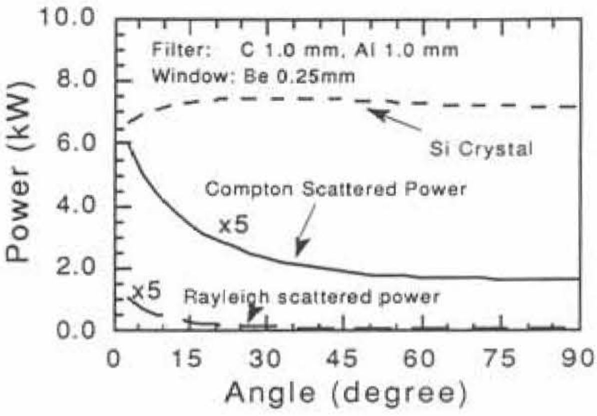

Fig.5 Heat power for the first Si crystal and back scattered power in the SPring-8 MPW beamline.

Table 2 Absorbed power and re-emitted power for C-Al-Be-filters (W).

Filter	AP	P_b^c	P_t^c	P_b^r	P_t^r	HP
C (1.00mm)	2873	164	214	8	75	2411
Al (1.00mm)	3487	114	159	9	130	3075
Be (0.25mm)	60	20	28	0	3	9

AP: Absorbed Power. HP: Heat Power

Figure 4 shows the X-ray flux of the MPW, the flux after the graphite filter and the flux after the Al filter. The flux after the Be window is almost the same as the flux after the Al filter because the X-ray hits on Be window is of hard one. The X-ray transmitted out of the Be window will be injected on Si crystal with a given angle. The heat distributions on each filter or window are listed in **Table 2**. Here we can see most of the heat power is loaded to the first optical element, the graphite filter and the secondary filter, the Al filter. For the graphite filter, the soft X-ray is almost completely absorbed, while about 10% of the absorbed power is re-emitted out of the filter due to the Compton and the Rayleigh scatterings. For the Be window, the incident X-ray is dominantly in hard X-ray region and the Rayleigh and the Compton scatterings are significant and about 80% of the absorbed power is re-emitted out of the Be window. The Be window does not subject to large heat power. **Fig.5** shows the heat power and the re-emitted power due to the Compton and the Rayleigh scatterings from Si crystal for various incident angle to the Si surface. At small incident angle, the X-ray are easily scattered out of the material so that the heat power is increase with the incident angle. At the same time, the penetrated power will increase as the incident angle increases. Due to the two competition mechanism, the final heat power will firstly increase and then decreases as show in **Fig.5**. The re-emitted X-rays become the heat source for the secondary Si crystal. This was shown in the experiment of NE1 beamline at the Photon Factory.23)

We have performed the theoretical heat load calculation for the SPring-8 MPW. Filters can only absorb the X-ray of low energy side. If the user is interested in 10 KeV range X-ray, the high-Z element can not be used as filter because it will absorb the X-ray user interested in. In such a case, the heat load on the Si crystal will increase. The deformation of Si crystal due to the large heat load will influence the quality of the mono-energy X-ray. User may select a filter system depending on the wavelength region which they want to use. Thus, It is better to use a mirror to filter out high energy X-rays. Therefor the heat power of Si crystal will be reduced so that the deformation due to the heat load can be minimized. In such a way, the high quality monochromatic photons can be supplied to the users. But it is noted that to use mirror, there is limitation of energy less than few tens keV. If the user hope to use the energy more than few tens keV, we have to consider another kinds of filter to cut the low energy parts of the beam, otherwise, Si crystal will have to subject the large heat load.

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Key Words

Photoinization:

The ionization of a binding electron by the absorption of photons through a photon-material interaction, and the electron is excited to a continuum state.

Compton Scattering:

The scattered process of X-rays or gamma rays by an electron where the energy of X-rays or gamma rays is reduced due to the scattering.

Rayleigh Scattering:

The scattering process of X-rays or gamma rays by a charged particles (an electron or a nucleus), where the energy of X-rays or gamma rays does not change.