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Abstract.
It is proposed and implemented a simple method of calculating of the output of the diffracted real photons of bremsstrahlung and transition radiation from perfect crystals of arbitrary thickness up to a primary extinction lengths. It is shown that for small thickness of crystals and observation angles concerning the center of the diffraction of reflex, contribution of diffraction of real photon is comparable with the output of parametric X-radiation. Influence of experimental equipment characteristic on observed characteristics of radiation is discussed.

1. Introduction

Parametric X-ray radiation (PXR) generated by passing fast charged particles through crystals had been actively studied till the end of the last century (see, for example, [1] and references therein). The interest to this type of radiation was mainly due to looking for tunable compact sources of intensive X-ray radiation for medical applications as an alternative to storage rings. Nowadays it is considered to be established (see, for example, [2]), that the PXR intensity in perfect crystals is not sufficient for medical applications. However, studies aimed at increasing the radiation intensity through the use of multi-crystal target [3] and multiple passing of particles through a thin target in circular accelerators [4] are being discussed till today. There have been recent suggestions to use PXR in thin crystals for diagnosing of electron beams parameters [5], and a new result for a thin crystal [6], which is not described by PXR theory [1].

In the first approximation PXR can be considered as coherent scattering of its own electromagnetic field of a particle on the electron shells of periodically arranged atoms of a target [1]. Diffracted in crystal X-ray and γ-rays, born directly inside the target or on its surface can be spread in the same direction as PXR. In the first case we mean the diffracted bremsstrahlung (DBS), and in the second one we mean the diffracted transition radiation (DTR). Apparently, first contribution of diffraction of real photons in the radiation yield at the Bragg angles of perfect crystals was confidently observed in experiments [8] for the (111) reflection of a single crystal silicon and [9] for the (110) of a diamond crystal. In the last paper the method of calculating the contribution of real photon diffraction in crystals with a thickness much greater than the length of the primary extinction for the Laue geometry is proposed. This limitation methods [9] and availability of experimental data about PXR which are not described theoretically excluding diffraction of real photons, provide an opportunity to consider the study of the influence of real photons diffraction on the observable characteristics up-to-date and of importance.

2. Theoretical consideration

In the general case in the experiment all the mechanisms of generation of radiation at the Bragg angles are implemented at the same time, so we introduce the basic formulae and approaches for each of them that we used during the calculation, following mainly the work of [9]. As it was shown in several experimental studies (see, for example, [10] and references therein), the kinematic PXR theory describes the results of measurements for energy electrons from a few MeV to several GeV with an accuracy better than 10-15 %. Thats why in order to calculate the PXR yield we used the formula obtained in the kinematic approximation by [11]:

$$\frac{d^2N}{dZd\Omega} = \frac{\sum_\alpha \alpha\omega^3|\chi_{\mathbf{g}}|^2}{2\pi\varepsilon_0^{3/2}\beta(1-\sqrt{\varepsilon_0}\boldsymbol{\beta}\mathbf{n})}\left[\frac{(\omega\boldsymbol{\beta}-\mathbf{g})\mathbf{e}_{\mathbf{k}_\alpha}}{(\mathbf{k}_\perp+\mathbf{g}_\perp)^2+\frac{\omega^2}{\beta^2}\{\gamma^{-2}+\beta^2(1-\epsilon_0)\}}\right]^2. \tag{1}$$

Here and further we use the system of units $\hbar = m_e = c = 1$. $\varepsilon_o = 1-\omega_p^2/\omega^2$, where ω_p is plasma frequency of the medium. $\boldsymbol{\beta} = \beta\mathbf{n}_0$ is the electron velocity vector, $\mathbf{n}_0$, $\mathbf{n}$ is a unit vector in the direction of the incident electron and the emitted photon (with energy ω and momentum $\mathbf{k}$), $\mathbf{g}$ is a vector of the reciprocal lattice, $\mathbf{e}_{\mathbf{k}_\alpha}$ are polarization vectors, $\perp$ is an index denoting the projections of a plane perpendicular to $\mathbf{n}_0$. The other symbols we use are common. By $|\chi_{\mathbf{g}}|^2$ we denote the magnitude of:

$$|\chi_{\mathbf{g}}|^2 = |S(\mathbf{g})|^2\exp(-2W)\left[-\frac{\omega_p^2}{\omega^2}\frac{f(\mathbf{g})}{z}\right]^2. \tag{2}$$

In (2) $|S(\mathbf{g})|^2$ is a structure factor, $\exp(-2W)$ is Debye-Waller factor, $f(\mathbf{g})$ is Fourier component of the spatial distribution of the electrons in the atom of the crystal.

The divergence of the electron beam, the electrons multiple scattering in the crystal and other experimental factors were taken into account according to the procedure described in [12].

For medium-energy electron the radiation in the X-ray range of photon energy ($\omega \leq 100$ keV) except PXR, is generated through the mechanisms of the transition radiation (TR) and the bremsstrahlung (BS). The TR spectral and angular distribution at the vacuum-medium interface can be represented in the form [13]:

$$\frac{d^2I_{TR}}{d\omega d\theta_\gamma} = \frac{2e^2\theta^3}{\pi}\left|\frac{1}{\theta_\gamma^2+\gamma^{-2}} - \frac{1}{\theta_\gamma^2+\gamma^{-2}+\omega_p^2/\omega^2}\right|^2 \tag{3}$$

where θ_γ is a photon emission angle according to the direction of the electron.

It is known (see, for instance [7]), that the bremsstrahlung in a dense medium in the energy range $\omega \leq \gamma\omega_p$ is suppressed due to the effect of medium polarization, and the degree of inhibition depends on both the energies of the photon and electron, and the angle of a photon emission. Therefore we used the expression for the spectral-angular distribution of the soft component of the bremsstrahlung ($\omega \ll E_e$), obtained as a result in [14] and taken into account this effect.

$$\frac{d^2I_{BS}}{d\omega d\Omega} = \frac{\gamma^2}{\pi L}\frac{(1+\frac{\gamma^2\omega_p^2}{\omega^2})^2+\gamma^4\theta_\gamma^4}{(1+\frac{\gamma^2\omega_p^2}{\omega^2}+\gamma^2\theta_\gamma^2)^4}, \tag{4}$$

where L is the radiation length.

The angle θ_γ in expressions (3), (4) is measured from the direction of the electron motion. Whereas in the experiment it is measured the distribution of the resulting radiation yield $Y(\omega,\theta)$ depending on the observation angle θ with the aperture ϑ_c.

The spectral and angular distribution of bremsstrahlung at the depth t when multiple scattering of electrons is taken into account $d^2I_{BS}^*(\omega,\theta,\varphi,t)/d\omega d\Omega$ is determined by convoluting the expression (4) with the angular distribution of the electrons $P(t,\theta_e,\varphi_e)$ at this depth:

$$\frac{d^2I^*_{BS}(\omega,\theta,\varphi,t)}{d\omega d\Omega} = \int P(t,\theta_e,\varphi_e)d\Omega_e \int \frac{d^2I_{BS}(\omega,\theta_\gamma,\varphi_\gamma)}{d\omega d\Omega_\gamma} f(\mathbf{n},\mathbf{n}_e,\mathbf{n}_\gamma)d\Omega_\gamma. \tag{5}$$

Here $\mathbf{n}_e(\theta_e,\varphi_e)$ and $\mathbf{n}_\gamma(\theta_\gamma,\varphi_\gamma)$ are vectors describing the direction of electrons and photons in the laboratory frame of reference and in a system connected with the direction of motion of the electron, respectively. $\mathbf{n}(\theta,\varphi) = \mathbf{n}_e + \mathbf{n}_\gamma$ is a vector of the photon direction in the laboratory frame, and $f(\mathbf{n},\mathbf{n}_e,\mathbf{n}_\gamma)$ is a function describing the connection between these vectors, see [15] for details.

In the experiments it is measured the dependence of a radiation yield into a fixed collimator from the angle of the crystal orientation Θ or an angular distribution, that is the dependence of the yield from the angles θ accordingly the center of reflex. This dependence can be written as:

$$Y_{DTR}(\theta) = \int d\omega \int \frac{d^2I^*_{TR}}{d\omega d\Omega} R(\omega,\mathbf{n},\mathbf{g},\Theta_D)S^*(\omega,\mathbf{n},T)d\Omega. \tag{6}$$

$$Y_{DBS}(\theta) = \int_0^T dt \int d\omega \int \frac{d^2I^*_{BS}}{d\omega d\Omega} R(\omega,\mathbf{n},\mathbf{g},\Theta_D)S(\omega,\mathbf{n},t)d\Omega, \tag{7}$$

where $d^2I^*_{TR}/d\omega d\Omega$ is TR spectral-angular distribution, taking into account the divergence of the primary electron beam, $R(\omega,\mathbf{n},\mathbf{g},\Theta_D)$ reflecting the ability for the direction vectors $\mathbf{n}$ and $\mathbf{g}$, determined by the crystal orientation angles Θ and the location of the detector Θ_D, $S^*(\omega,\mathbf{n},T)$ and $S(\omega,\mathbf{n},t)$ are functions taking into account the photons absorption in the crystal and the geometry of the experiment, T is thickness of the crystal. The integration into (6), (7) is taking place over all angles and photon energies with the hit of the photons in the collimator.

3. Description of the computational model

To determine the output of the diffracted radiation we need information about $R(\omega,\mathbf{n},\mathbf{g},\Theta_D)$. The work [9] is based on the fact that if the thickness of perfect crystals T, significantly exceeding the primary extinction length l_{ex}, then in a narrow angular cone $\Delta\Theta$ (in so-called Darwins table) near the Bragg direction in absence of absorption reflectivity is equal to 100%, while outside of this range it is negligible [16]. Therefore, as a result of photons multiple reflections in a crystal of big thickness ($T \gg l_{ex}$) at any point of it a half of the radiation that satisfies the Bragg condition is spreading along the initial direction, and the other half in the Bragg direction.

According to this approach for a fixed photon direction $\vec{n}$ from the beam with the spectral-angular distribution of $d^2I^*_{BS}/d\omega d\Omega$ or $d^2I^*_{TR}/d\omega d\Omega$ satisfying Bragg's condition for photons with energies of ω only photons in the energy range $\Delta\omega = \omega\cos(\Theta_B)/\sin(\Theta_B)\Delta\Theta$ will be reflected. In accordance with [16] for unpolarized radiation and lack of absorption $\Delta\Theta = 2\cdot\gamma\Delta\theta_0$, where $\Delta\theta_0 = 2\cdot\delta/\sin 2\Theta_B$ is an amendment to the Bragg angle Θ_B because of the refraction of waves in a crystal, $\delta = (\omega_p/\omega)^2/2$ is a difference between the refractive index from 1, and $\gamma = f(\mathbf{g})(1+\cos(2\Theta_B))/2f(0)$.

As an estimate of the characteristic parameter of the model that is the length of the primary extinction we can use the expression [16]:

$$l_{ex} = d/(2\bar{\xi}\sin\Theta_B), \tag{8}$$

where d is a distance between planes, and $\exp(-2\bar{\xi})$ is an impairment of the intensity of the primary wave as it passes through a plane with the reciprocal lattice vector $\vec{g}$:

$$2\bar{\xi} = \frac{\pi d^2 NS(\mathbf{g})f(\mathbf{g})}{n}\frac{e^2}{mc^2}, \tag{9}$$

where N is a concentration of the scattering centers, n is the order of reflection.

To calculate the reflectivity $R(\omega, \mathbf{n}, \mathbf{g}, \Theta_D)$ we use three of the coordinate system proposed in [17], in which Z-axis of two of them is turned around a vertical axis concerning Z axis of the laboratory system, right on the angle Θ_D (system of a "detector") and $-(\pi/2 + \Theta_B)$ (system of "a crystal"). The boundary directions of hit of radiation in the collimator $\theta_x, \theta_y, \theta_z$ are given in the system of "a detector". By means of transition into a system of "a crystal" we define the direction of movement of the photons after reflection. As in the system of "a crystal" the reflection of photons is equivalent to changing the sign of θ_z, after such transformation we learn the direction of motion of photons prior to diffraction.

The transition from the system of "a detector" into the laboratory system gives us an opportunity to determine the direction of the photons which can reach the detector after the process of diffraction and find the diffracted emission yield. The photon energy and intensity of the reflected radiation is determined in accordance with Bragg's law and the expressions of (3)-(7). The integration of equations (5)-(7) to obtain the final angular distribution or orientation dependence of the radiation yield for each order of reflection is performed numerically.

As it is noted in [18], in crystals with weak absorption the establishment of a stationary mode of transmission of photons through the crystal required for the legitimacy of the use of techniques [9], occurs for a photon path in a crystal of about 10 l_{ex}. A typical value of the primary extinction length is about 10 microns, while we have observed quite differences from the predictions of the PXR theory with a crystal thickness of 50 μm [5] and 20 μm [6].

For the part of the crystal with a thickness much smaller than l_{ex}, the probability of reflection of photons with an energy of ω and direction $\mathbf{n}$, for which the Bragg condition is satisfied, is proportional to the number of planes crossed by them [16]. Therefore, the dependence of the number of photons, which have not undergone the reflection, on the way length in the crystal t can be written as $N_\gamma(t) = N_\gamma(0)\exp(-t/l_{ex})$ [16], where $N_\gamma(0)$ is the number of photons at a starting point. The possibility of such notation allows us to use a well-known in experimental physics method of statistical simulation of photon transmission through a matter and for the conditions of photon diffraction in perfect crystals, as it was done in [19] for mosaic ones.

Taking into account the multiple Bragg reflection, photon absorption and scattering on atoms the dependence of the number of photons on passable way can be rewritten in the following way:

$$N_\gamma(\omega, \mathbf{n}, t) = N_\gamma(0)\exp(-\mu_{tot}(\omega, \mathbf{g}, \mathbf{n})t), \tag{10}$$

where $\mu_{tot}(\omega, \mathbf{g}, \mathbf{n}) = \mu(\omega) + \mu_{dif}(\omega, \mathbf{g}, \mathbf{n})$ is a total coefficient of linear absorption of radiation with energy ω, for the direction of the reflecting plane of the crystal $\mathbf{g}$ and the direction of the photon velocity $\mathbf{n}$. We consider $\mu(\omega)$ as a linear absorption coefficient of photons due to the all processes on separate atoms and $\mu_{dif}(\omega, \mathbf{g}, \mathbf{n}) = 1/l_{ex}(\omega, \mathbf{g}, \mathbf{n})$ is due to diffraction.

The process of photons propagation through a crystal was being simulated in the following way. There were defined the values $\mu(\omega)$ and $\mu_{dif}(\omega, \mathbf{g}, \mathbf{n})$ for the photon with the energy of ω and the direction of motion $\mathbf{n}$ satisfying the Bragg condition. Then it was played out the photon path to the interaction point $t = -\ln\xi/\mu_{tot}$, where ξ is a random number between zero and one. Then the coordinates of the interaction point were being determined. If the point didn't belong to the crystal, the process with the photon was over and the new process started again.

If the interaction occurred inside the crystal, then we found out what kind of process took place. We were interested if it was diffraction or any other process on a separate atom. In the last case, the process with the photon was over and the new process started again. In the case of diffraction, the simulation was being repeated until the photon left the crystal or absorbed in it. This method is not limited concerning thickness and geometry of a using crystal.

4. Comparison of the calculated results with the experimental data

As it is noted above, the main and true objective of the article is, firstly, the analysis of results of new experimental works, in which the contribution of diffraction of real photons into an output of resulting radiation has become of great importance and secondly, the development of the calculation procedure, giving us an opportunity to consider the contribution of diffraction of real photons in crystals of any thickness. In order to define limits of applicability of a technique [9] it was carried out a number of calculations of an output of the diffracted radiation from thin crystals with the use of both the technique [9], and the one described above, which takes into account more correctly repeated Bragg's reflection of photons inside a perfect crystal.

Vertical angular distribution PXR of is represented in figure 1 (∘), distributions of the DTR and DBS and their sum for experimental conditions [6] and the first order reflection calculated by a technique [9], so these are the curves 1-3. The ratio of the DTR angular distributions, calculated by both techniques, is also represented in the figure.

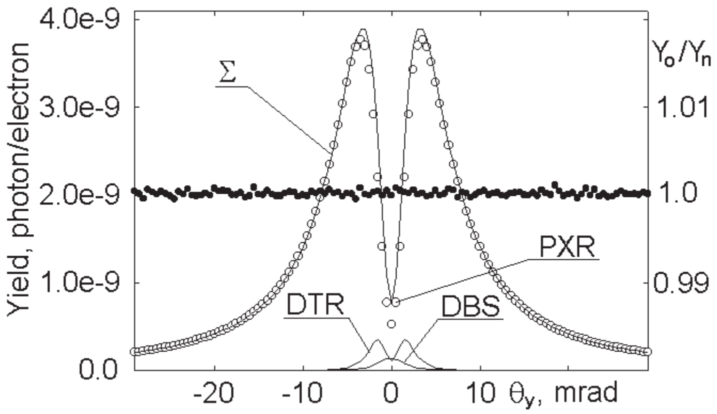

Figure 1. Vertical distribution of the X-ray yield for [6] condition and the first reflection order. • - ratio calculated DTR yields for both techniques

As can be seen from the figure, PXR has bigger intensity than DBS and DTR, and its angular distribution is broader. In the center of PXR angular distribution there is a dip, whereas the output of DTR and DBS is concentrated near the Bragg's direction. As a result, the diffracted photons yield gives the main contribution into the radiation yield in the reflex center.

The ratio of DTR yields, calculated by means of both techniques, is not different from 1, and the straggling concerning it, is caused by statistics of simulation. According to (8) for ω=11.65 keV and reflection (220) the length of primary extinction in silicon is $l_{ex} \sim 5\ \mu$. That is a simpler technique [9] can be used up to thickness of crystals of $T \sim$ 4-5 l_{ex}. The distinction of angular distributions, calculated by both techniques, begins with the a crystal thickness of $T \sim 2\ l_{ex}$.

In the paper mentioned above [5], [6] measurements of radiation angular distributions were carried out by means of the ProxiVision HR25 X-Ray camera [5] and the position-sensitive detector on a basis, of so-called, imaging plate (IP)[6]. In other words, as a matter of fact it wasn't measured an angular distribution of a photon beam, but a response of a detector on the energy of radiation which arrived on it. The first device registers the light output in this or that point of a thin scintillating plate at hit of a X-ray beam on it; as for the second one, it measures the absorbed dose in this or that point of the IP.

The results of calculation of horizontal angular distributions of resultant radiation are represented in figure 2, these are PXR+DTR+DBR for three orders of reflection and conditions of experiments [5], [6], see figures 2a and 2b. So for the reasons stated above, we summed up not the angular distributions of photons, but the angular distributions of intensity of radiation.

As can be seen from figures, the contribution of real photons diffraction significantly increased the yield of radiation in a minimum of PXR angular distribution (see fig.1). Nevertheless the output of radiation in a minimum of calculated dependence $\sim$ 40% from a maximum for figure 2a and $\sim$ 55% for figure 2b, is less than in the cited works, $\sim$ 50% and $\sim$ 75%, respectively. We believe that more consistent accounting of the experimental equipment characteristics and experiment layout will lead to an accord of experimental and calculated results.

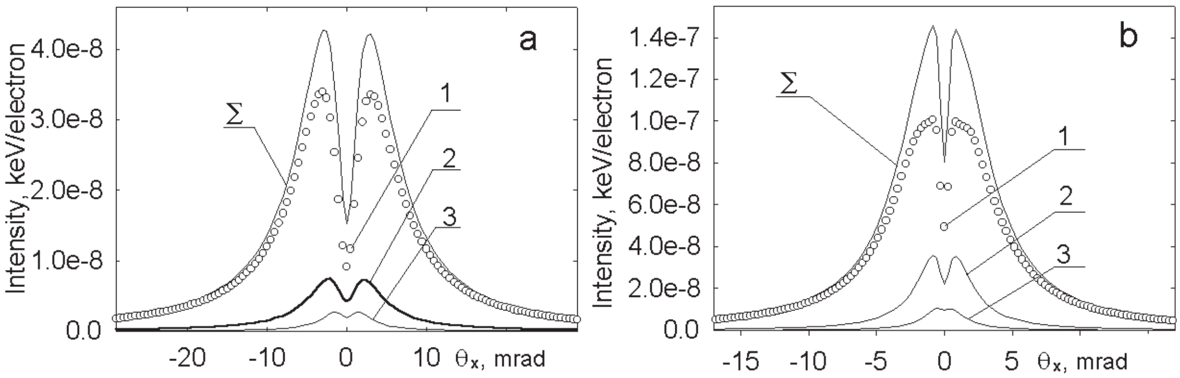

Figure 2. Horizontal angular distribution of X-ray intensity for three reflection orders and the experimental condition [6] (fig. 2a) and [5] (fig. 2b).

5. Summary and Conclusions

The results of the present research could be briefly stated as follows:

1) It is proposed and implemented a simple method of calculating of output of diffracted real photons in perfect crystals of arbitrary thickness up to the primary extinction lengths.

2) The method of computing of the contribution of diffraction of real photons, proposed in the work [9] is efficient up to the thickness of the crystals of an order of several lengths of primary extinction.

3) In order to explain the experimental results [5], [6] you should rationally take into account the characteristics of the used registration equipment.

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