Laser induced x-ray radiation under the grazing incidence geometry

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Abstract. In conventional schemes of the parametric x-ray radiation (PXR) the beam of charged particles moves through the crystal and destruction of target and beam takes place. It is possible to avoid the destruction and to increase the interaction length if the scheme of grazing incidence diffraction (GID) is used: the beam of charged particles propagates in vacuum near the crystal surface while the photons are emitted under conditions of GID. In this case a highly collimated and precisely positioned beam is required. The restrictions on beam parameters can be avoided if intense laser radiation is backscattered by the electron beam. In the paper a theory of laser induced x-ray radiation under conditions of grazing incidence diffraction is presented and distributions of emitted quanta are calculated. Properties of the radiation and possible applications are discussed.

1. Introduction

One of the ways to get higher output of the parametric x-ray radiation (PXR) is to increase the interaction length and beam current. These parameters could be much higher if electrons move along the surface of the crystal without penetrating it. To obtain PXR output from such electrons the structure of eigen electromagnetic field near crystal should have a wave propagating at grazing angle to the surface. This kind of the electromagnetic field belongs to special cases of electromagnetic fields considered in the x-ray diffractometry (XRD) for which traditional two-wave simplification of the dispersion equation is not valid and additional roots and waves should be taken into consideration [1].

There are two main special cases of XRD: extremely asymmetric diffraction (EAD) and grazing incidence diffraction (GID). In case of EAD diffracted (or incident) wave makes a grazing angle to the surface and it is necessary to consider the reflected wave also. It should be mentioned that the pioneering PXR experiments in Tomsk were done in this geometry and were completely described theoretically [2], [3].

The second case is GID. It is widely used nowadays in XRD (due to its surface sensitivity). Here the reciprocal space vector lies in the plane of crystal surface and all waves propagate at grazing angles. In this conditions reflected waves play essential role and complete fourth-order dispersion equation should be used. The spectral-angular distribution of PXR in GID geometry was considered before in the series of the papers [4] - [6]. The integral characteristics of PXR under GID geometry (GID-PXR) in dependence of the electron beam parameters and the influence of the external radiation source (laser field) on the GID-PXR properties are considered in the present paper.
2. Calculation of GID-PXR intensity

Consider the next experimental geometry: high-energy electrons move almost parallel to the crystal surface, the distance between the beam and the surface is \( z_0 \), the velocity vector \( \vec{v} \) is inclined on angle \( \alpha \) against the surface and makes angle \( \theta_B \) with considered set of crystallographic planes (Figure 1). Under this conditions PXR is concentrated along the direction of vector \( -\vec{k} \), which is parameterized via out-of-plane angle \( \phi \) and in-plane deviation \( \theta \). The wave vector \( \vec{k} + \vec{h} \) of the diffracted wave is almost antiparallel to the electron velocity \( \vec{v} \). Under such conditions no destruction of the crystal and the beam are occurred. It enables to increase the interaction length from the absorption length, which is typical for the conventional schemes of PXR, to the crystal size. Also, it becomes possible to generate PXR directly inside the accelerator ring and to take advantage of high current and high energy of particles there [4], [7].

The spectral density of PXR can be calculated on the basis of classical electrodynamics according to the next formula [8], system of units \( \hbar = c = 1 \) is used:

\[
W_{\vec{n}\omega s} = \frac{\omega^2}{4\pi^2} \left| \int d^3\vec{r} \vec{J}_\omega(\vec{r}) \vec{E}_{k\omega s}^{(-)}(\vec{r}) \right|^2 ,
\]

where \( \vec{n} = -\vec{k}/k \) is the unit vector directed towards the detector of radiation, \( \vec{J}_\omega(\vec{r}) \) is the temporal Fourier-transform of the beam current, index \( s = \sigma, \pi \) defines the radiation polarization. \( \vec{E}_{k\omega s}^{(-)}(\vec{r}) \) is the electric field of the time-reversed eigen wave which satisfies the homogeneous Maxwell equations taking into account the presence of crystal and the boundary conditions \( e_s e^i\vec{k} r \) at the detector side [8]. It replaces the plane wave in vacuum electrodynamics and accounts for interaction with the media.

In order to find out the field \( \vec{E}_{k\omega s}^{(-)}(\vec{r}) \) the XRD problem should be solved. When the incoming wave vector \( \vec{k} \) is close to the Bragg condition for the reflex defined by the reciprocal lattice vector \( \vec{h} \) the two-wave approximation can be used, which leads to the next structure of the electric field above the crystal:

\[
\vec{E}_{k\omega s}^{(-)}(\vec{r}) = \vec{e}_{k_s} T_0 e^{i\vec{k} \cdot \vec{r}} + \vec{e}_{R} Re^{i\vec{k} \cdot \vec{r}} + \vec{e}_{h} He^{i\vec{k} \cdot \vec{r}} ,
\]

where \( T_0 = 1 \), \( R \), \( H \), are the amplitudes of the incident, reflected, diffracted waves; \( \vec{k}, \vec{e}_{k_s}; \vec{k}_R, \vec{e}_{k_R}; \vec{k}_h, \vec{e}_{k_h} \) are the wave vectors and unit polarization vectors correspondingly. In the chosen reference frame, wave vectors components are following:

\[
\vec{k} = \{-h_x, 0, 0\}; \quad \vec{k}_R = \{\vec{k}_\parallel, -\omega \gamma_0\}; \quad \vec{k}_h = \{\vec{k}_\parallel + \vec{h}, -\omega \gamma_h\};
\]

\[
\vec{k}_\parallel = \omega \{\cos \varphi \sin (\theta_B + \theta), \cos \varphi \cos (\theta_B + \theta), 0\}; \quad \gamma_0 = \sin \varphi.
\]

\[\text{Figure 1. GID-PXR geometry, see text for the details.}\]
Here $\vec{h}$ is assumed to belong the interface plane (Figure 1), i.e. no miscut is considered. From the condition $k = k_R = k_h = \omega$ the useful relation between $\gamma_0$ and $\gamma_h$ follows

$$\gamma_h = \sqrt{\frac{\gamma_0^2}{\gamma_0^2 - \alpha}}, \quad \alpha = \frac{2\vec{k} \cdot \vec{h} + h^2}{\omega^2},$$  \hfill (4)

where $\alpha$ is deviation from Bragg condition.

To find the wave field inside the crystal, consider the wave field in the form of

$$\vec{D}_0(\vec{r}) = \sum_i D_i(\vec{e}_{k,i} e^{i(\vec{k} \cdot \vec{r} + \omega u_i \zeta)} + \bar{v}_i \vec{e}_{k,s,i} e^{i(\vec{k} \cdot \vec{r} + \omega u_i \zeta)}),$$  \hfill (5)

where the longitudinal wave vector component $\vec{k}_l$ is the same as above, the interface due to boundary conditions and the value $u_i$ describes the wave refraction. The values $v_i$ and $u_i$ can be found from a system of algebraic equations which follows from the Maxwell equations taking into account crystal susceptibilities $\chi_0,\chi_h,\chi_{-h}$ in the two-wave approximation:

$$ (u^2 - \gamma_0^2 - \chi_0) - v C \chi_{-h} = 0; \quad (u^2 - \gamma_h^2 - \chi_0) v - C \chi_h = 0,$$  \hfill (6)

where $C = 1$ for $\sigma$ polarization and $C = \cos 2\theta_B$ for $\pi$ polarization. The condition of nontrivial solution of (6) provides the dispersion equation of the fourth-order for the value $u$, which can be solved here analytically; after $u_i$ is known, $v_i$ are found trivially:

$$u_{1,2} = \sqrt{\frac{\gamma_0^2 + \chi_0 - \alpha \pm \sqrt{\alpha^2 + 4\gamma_0^2 \chi_h \chi_{-h}}}{2}}, \quad v_{1,2} = \frac{u_{1,2}^2 - \gamma_0^2 - \chi_0}{C \chi_{-h}},$$  \hfill (7)

the solutions $u_{3,4} = -u_{1,2}$ are not considered as they do not agree with boundary conditions.

To determine the wave filed completely, the amplitudes $R, H, D_1, D_2$ should be found from the boundary conditions. In the case of x-rays standard conditions for magnetic and electric field are reduced to the continuity conditions for amplitudes and their derivatives for each longitudinal wave vector. With definitions (2), (5) we obtain:

$$1 + R = D_1 + D_2; \quad \gamma_0(1 - R) = u_1 D_1 + u_2 D_2; \quad H = v_1 D_1 + v_2 D_2; \quad -\gamma_h H = u_1 D_1 + u_2 D_2.$$  \hfill (8)

For the calculation of the PXR intensity only the diffracted wave $\vec{e}_{k,h} e^{i\vec{k}_h \cdot \vec{r}}$ is of interest, its amplitude is found from (8):

$$H = \frac{2(u_1 - u_2) v_1 v_2 \gamma_0}{((v_1 - v_2)(u_1 u_2 + \gamma_0 \gamma_h) + (u_1 v_1 - u_2 v_2) \gamma_0 + (u_2 v_1 - u_1 v_2) \gamma_h)},$$  \hfill (9)

and unit polarization vectors can be chosen as

$$\vec{e}_\sigma = \vec{k} \times \vec{k}_h / \| \vec{k} \times \vec{k}_h \|, \quad \vec{e}_\pi = \vec{e}_\sigma \times \vec{k}_h / \| \vec{e}_\sigma \times \vec{k}_h \|.$$  \hfill (10)

The second important term in the equation for PXR spectral density is the spectral density of beam current. Consider the next model parameters describing the beam: small angle $\alpha$ between electron velocity and crystal surface, mean distance between the beam and the surface $z_0$, beam width (dispersion of beam position) $\sigma_z$. Suppose also that inclination angle $\alpha$ and beam position $z_0$ are interconnected through a parameter $\delta_{z,\alpha}$ called emittance. Then the beam current spectral density normalized on one electron is:
\[ j_{\omega}(\mathbf{r}) = \frac{e}{2\pi} \int dt dz \frac{1}{\sqrt{\pi} \sigma_z} \exp \left( -\frac{(z - z_0)^2}{\sigma_z} \right) e^{i\omega t} \delta(\mathbf{r} - \mathbf{v}_t - \mathbf{r}_0). \] (11)

After inserting field and current in the spectral density expression and integrating over the frequency we obtain the next expression for angular distribution of PXR photons:

\[
\frac{\partial^2 N_\omega}{\partial \theta \partial \varphi} = \frac{\alpha}{2\pi} L_c \omega^2 |H(\theta, \varphi) \mathbf{e}_\varphi \mathbf{v} B|^2 \\
B = \frac{1}{2} e^{i\omega\gamma_z} \left[ \sigma_z \left( \frac{z_0}{\sigma_z} + \frac{1}{2} i \omega \gamma \sqrt{\frac{\sigma_z}{2}} \right) \right],
\] (12)

where \( L_c \) is the coherent length that is equal here to the crystal length, \( B \) is the factor originating from distribution in \( z \) direction, \( \text{Erfc} \) is the error function, \( \alpha = 1/137 \) is the fine structure constant.

The PXR frequency \( \omega \) is found from a Cherenkov-like condition \( \delta(\omega - k_h \mathbf{v}) \) and has the following form:

\[
\omega = \frac{h \beta \cos \alpha_v \sin \theta_B}{1 - \beta \cos \alpha_v \cos (2\theta_B + \theta) \cos \varphi},
\] (13)

From the dispersion equation for electromagnetic field in vacuum the next expression for the diffracted wave vector component normal to the surface follows

\[
\omega \gamma_h = \sqrt{\omega^2 \sin^2 \varphi - h^2 + 2h_x \omega \cos \varphi \sin (\theta_B + \theta)},
\] (14)

This component proved to be always imaginary. It means that intensity from a single electron decreases exponentially when the distance from the crystal surface increases, the typical distance of attenuation can be estimated as

\[
z_0 \sim \frac{\lambda_{\text{x-ray}}}{\sqrt{1/\gamma^2 + \alpha_v^2}}.
\] (15)
However, for a beam of particles with Gaussian distribution this dependence is described by factor B in (12) and is not so strong. Figure 2 shows the dependence of the factor B on the distance of beam center from the surface for electron energy $E = 5\text{GeV}$ and $\sigma_z = 0.3z_0$, $\theta_B = \pi/3$, reflex (220) of Si crystal (this parameters are used below as well) at angles $\theta = 0$, $\varphi = \sqrt{|\chi_0|}$, $\alpha_v = 0$. For comparison the curve calculated for infinitely narrow beam is also shown. One can see that for these realistic parameters PXR intensity decreases rapidly with distance $z_0$ and in case of beam with distribution in $z$ mainly the "tail" of the distribution close to the interface contributes to PXR formation. Hence, the alignment of the beam as close as possible to the crystal surface is of primary importance.

The dependence on beam emittance comes out to be very strong. Actually, at given beam position $z_0$ the emittance determines the coherent length and normal wave vector component that enters the factor B. Figure 3 shows dependence of PXR intensity at maximum on beam distance from crystal for two values of emittance. One can see that increase of one order in emittance causes many orders of decrease in intensity.

One of distinctive PXR features is narrow angle and spectral distribution. Figure 4 shows the angular distribution of PXR photons density for $\sigma$ and $\pi$ polarizations calculated for (220) reflex of Si crystal. The width of peak in out-of-plane direction has the order of $\sqrt{|\chi_0|}$ that is typical for GID, the width in in-plane direction depends on factor $\gamma = E/m$ and angle $\alpha$. The absolute value of intensity depends greatly on beam emittance.

3. Laser induced GID-XR radiation

From mathematical point of view, to overcome the exponential dependence on the distance from crystal one can add a small additional item in the Cherenkov-condition. It would make the normal wave vector component real in some angle area and remove the dependence of intensity on beam distance. Physically, it corresponds to some periodical influence. For example, consider an external linearly-polarized laser field $\vec{E}(\vec{r}, t) = \vec{E}_0 e^{i(k_z r - \Omega t)}$ of optical frequency $\Omega$ acting on the electron. This field makes the electron to move with the oscillating velocity $\vec{u}$.

**Figure 4.** Angular distribution of PXR photon density for $\sigma$ and $\pi$ polarizations for $L_c = 0.1\text{cm}$, $\alpha_v = 10^{-3}\text{rad}$, $z_0 = 1\mu\text{m}$, Si crystal, reflex (220).
\[ \vec{v}(t) = \vec{v}_0 + \vec{u} e^{-i\Omega(1+\beta)t}; \quad \vec{u} = \frac{eE_0}{\gamma m\Omega}, \]  
(16)

the resulting law of motion being

\[ \vec{r}(t) = \vec{r}_0 + \vec{v}_0 t - \frac{\vec{u} e^{-i\Omega(1+\beta)t}}{i\Omega(1+\beta)} ; \]  
(17)

Inserting the law of motion obtained in the expression for the beam current and performing the integration over frequency in general expression for spectral-angular distribution we get the next angular distribution of emitted XR quanta:

\[ \frac{\partial^2 N_s}{\partial \theta \partial \phi} = \frac{\alpha \omega}{2\pi} L_c \omega \left| H(\theta, \phi) \vec{e}_{k_{hs}} \left( \vec{u} - \vec{v}_0, \frac{k_h \vec{u}}{\Omega(1+\beta)} \right) e^{i\omega \gamma z_0} \right|^2 \frac{1}{1 + k\vec{v}_0^2} \]  
(18)

The frequency of electron oscillations \( \Omega(1+\beta) \) enters the Cherenkov-condition which has the form \( \delta(\omega + k_h \vec{v} - \Omega(1+\beta)) \). The frequency of emitted XR photons is

\[ \omega = \frac{h_x \beta \cos \alpha \cos \theta_B + \Omega(1+\beta)}{1 - \beta \cos \alpha \cos (2\theta_B + \theta) \cos \phi}, \]  
(19)

and is slightly changed compared to (13). This change makes the value of normal wave vector component (14) real when the in-plane angle \( \theta \) is less than \( \theta_{cr} \) equal to

\[ \theta_{cr} = \sqrt{2 \left( \frac{\Omega(1+\beta)}{\omega_B} - \frac{1}{2\gamma^2} \right)} . \]  
(20)
For optical range of laser frequency the necessary electron energy has order of tens MeV, and the dependence on beam collimation becomes quite weak.

This behavior can be understood if we consider the process of XR quanta emission as Compton backscattering of laser photons and their diffraction in crystal. The photons are generated in vacuum and the crystal acts like a monochromator.

The angular distribution is presented on Figure 5. It has two almost symmetric maxima placed at in-plane angle $\theta_{cr}$ (Figure 5; left panel). The width of the peaks in both directions has the order of $\sqrt{|\chi_0|}$. The shape of the peak is typical for GID diffraction (Figure 5; right panel). The absolute value of XR intensity is proportional to square of induced velocity and hence to the laser power density. For the parameters used the quantum yield of x-ray quanta is approximately $10^{-11}\text{ photons/electron}$. For more powerful laser it will be higher, correspondingly.

4. Conclusions

A new scheme for generation of parametric x-ray radiation is proposed. The beam of ultrarelativistic charged particles propagates in vacuum near the crystal surface while the photons are emitted under conditions of GID. Under such conditions no destruction of crystal and beam takes place. Hence, the interaction length can be increased to the lateral size of the crystal and no restrictions on beam current are imposed. However, the analysis shows that ultra relativistic electrons are required (tens GeV) and GID-PXR is very sensitive to beam position and emittance. This sensitivity can be utilized to perform the transverse beam profile diagnostics, such application will be discussed elsewhere.

Application of the laser field enables to avoid strong dependence on the beam parameters and to obtain XR quanta at electron energies of tens MeV. The intensity of XR then becomes proportional to the laser power density.

A promising application of GID-PXR is construction of a diffraction resonator without the absorption of the emitted photons. It can enhance parametric beam instability [9] and lead to the coherent radiation in the x-ray range.

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