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Spectral-angular characteristics of surface parametric x-ray radiation of a relativistic electron

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Abstract. The spectral-angular characteristics of the surface parametric x-ray radiation (SPXR) of an electron, moving at a small angle to the crystal surface, are found. The distribution of quanta, considering the formation of the radiation both in vacuum and in a medium are obtained. The characteristics of SPXR for a number of crystal reflections with the diamond-type structure (Ge, Si and C) are calculated.

1. Introduction

At present, the parametric x-ray radiation (PXR) effect, caused by a relativistic particle uniformly moving in a crystal, is being actively studied [1–5]. It is shown in [6] that, as a charged particle passes in vacuum over the surface of a space-periodic medium, radiation of a new type occurs, which is called parametric quasi-Cherenkov radiation. If the medium is a crystal, the radiation frequency is over the x-ray spectral range. One of the interesting features of surface parametric radiation is its possibility of exciting a surface wave owing to dynamic interaction of an electron field with a crystal [6]. the surface wave [7] appears under conditions of total external reflection of x-ray radiation in the case of grazing-geometry diffraction, which was first theoretically considered in [8] and experimentally studied in [9–12].

The theory of surface parametric radiation for the case of particle motion parallel to the surface of a periodic medium was presented in [6]. In the present work the spectralangular distribution of quanta from the surface parametric x-ray radiation (SPXR) is found, when the particle moves at a small angle to the crystal surface. The results of numerical calculations of basic radiation characteristics for the given reflection of a germanium single crystal are given. A comparison is made of the spectral and the angular distributions of SPXR for a number of single-crystal reflections with the diamond structure (Ge, Si and diamond). The conditions for experimental observation of the radiation described are considered.

2. SPXR of a relativistic electron: basic formulae

Let us consider radiation from an electron, passing through the semi-infinite crystal at a small angle $\theta_0 \ll 1$ with its surface. Let one of the reciprocal lattice vectors of a crystal

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Figure 1. Grazing geometry diffraction of a plane wave with a wavevector k_0 in a number of (hkl)planes with a corresponding reciprocal lattice vector $2\pi\tau$, parallel to the surface.

 $2\pi\tau$ make a small angle $\psi < |\chi_0|^{1/2}$ (χ_0 is the dielectric susceptibility) with this surface and an arbitrary angle with the tangent electron velocity component.

According to [6, 13], the spectral density of the radiation energy per unit of solid angle in the n = k/k direction (k is the photon wavevector in vacuum) is determined by the expression

$$W_{n\omega} = \frac{\omega^2}{4\pi^2 C^3} \sum_{s} \left| \int E_{ks}^{(-)*}(r,\omega) \, \mathrm{d}^3 r \right|^2 \tag{1}$$

where s is the photon polarization index, $j = (r, \omega)$ is the Fourier image of the electron current density, $E_{ks}^{(-)*}(r, \omega)$ relates to the solution of the homogeneous Maxwell equations of $E_{ks}^{(+)*}(r, \omega)$, which describe the diffraction of a photon on the crystal surface by the relation

$$E_{ks}^{(-)*} = E_{-ks}^{(+)}.$$
(2)

The electron current density is

$$j(\mathbf{r},t) = ev\delta(\mathbf{r} - \mathbf{r}(t)) \tag{3}$$

where e is the charge, v is the velocity and r(t) is the electron trajectory. Having substituted (3) into (1), we get the spectral-angular distribution for the number of quanta which have escaped:

$$\frac{\partial^2 N_s}{\partial \omega \,\partial \Omega} = \frac{W_{n\omega}}{\hbar \omega} = \frac{e^2 \omega}{4\pi^2 \hbar c^3} \left| \int v \cdot E_{ks}^{(-)*}(\mathbf{r}(t), \omega) \exp(i\omega t) \,\mathrm{d}t \right|^2. \tag{4}$$

To find $E_{ks}^{(-)*}$, we shall consider the dynamical surface diffraction of x-ray radiation in the geometry, proposed in [8]. Let a plane wave, having a wavevector of $k_0 = (k_{0t}, k_{0z})$ be incident on a crystal (figure 1). At small angles of incidence, besides a specularly reflected wave with a $k'_0 = (k_{0t}, -k_{0z})$ vector, a diffracted reflected wave emerges in vacuum, whose wavevector tangent component differs from the incident wave by the reciprocal lattice vector, i.e. $k_{rt} = k_{0t} + 2\pi\tau$. Then the field in vacuum may be written as

$$E_{ks}^{(+)v} = e_s \exp[i(k_{0t} \cdot r_t + k_{0z}z)] + A \exp[i(k_{0t} \cdot r_t - k_{0z}z)] + B \exp[i(k_{\tau t} \cdot r_t - k_{\tau z}z)]$$
(5)

where $k_{\tau z} = \sqrt{k_0^2 - k_{\tau t}^2}$.

The field in a medium satisfies the Maxwell equations, which in the two-beam approximation of the dynamical diffraction theory reduce to the following set of equations, relating Fourier components of transmitted E(k) and diffracted $E(k_t)$ fields:

$$\begin{aligned} (k^2/k_0^2 - 1)E(k) &= \chi_0 E(k) + \chi_{-\tau} E(k_{\tau}) \\ k_{\tau}^2/k_0^2 - 1)E(k_{\tau}) &= \chi_{\tau} E(k) + \chi_0 E(k_{\tau}) \end{aligned}$$
(6)

where $k_r = k + 2\pi\tau$, $\chi_{0,\pm\tau}$ are coefficients of the expansion of a crystal dielectric susceptibility into Fourier series versus reciprocal lattice vectors. For σ and π polarizations $(e_{\sigma} || e_{\sigma\tau} || [k \cdot k_r], e_{\pi} || [k \cdot e_{\sigma}], e_{\pi\tau} || [k_r \cdot e_{\sigma\tau}])$, (6) divides into two independent sets of scalar equations. Further we shall discuss only the radiation for the π polarization. From the condition of solvability of (6) for this polarization it follows that

$$k_{1(2)z} = k_0 (k_{0z}^2 / k_0^2 + \chi_0 - \alpha/2 \pm \frac{1}{2} \sqrt{\alpha^2 + 4\chi_{\tau\pi}\chi_{-\tau\pi}})^{1/2}$$
(7)

where $\chi_{\pm\tau\pi} = \chi_{\pm\tau}(e_{\pi} \cdot e_{\pi\tau})$, $\alpha = (2k_0 \cdot 2\pi\tau + 2\pi\tau^2)/k_0^2$ is the parameter characterizing the deviation from the exact Bragg condition. The field in a medium may be written in the form

$$E_{k\pi}^{(+)m} = \sum_{\mu=1,2} e_{\pi} E_{\mu} \exp[i(k_{0t} \cdot r_{t} + k_{\mu z} z)] + e_{\pi\tau} E_{\mu} c_{\mu} \exp[i(k_{\tau t} \cdot r_{t} + k_{\mu z} z)]$$
(8)

where

$$c_{1,2} = 2\chi_{-\tau\pi} / [\alpha \pm (\alpha^2 + 4\chi_{\tau\pi}\chi_{-\tau\pi})^{1/2}].$$

At small angles of photon incidence equal to $|\pi/2 - \theta| \sim |\chi_0|^{1/2}$, i.e. when they are of the order of the critical angle of total external reflection, and when $\psi < |\chi_0|^{1/2}$, the difference between the diffraction plane and the crystal surface may be neglected. Boundary conditions in this case can be given by

$$(E_k^{(+)v})_t = (E_k^{(+)m})_t \qquad (\operatorname{rot} E_k^{(+)v})_t = (\operatorname{rot} E_k^{(+)m})_t. \tag{9}$$

We obtain the following expressions for amplitudes:

$$A = [c_1(k_{0z} - k_{2z})(k_{\tau z} + k_{1z}) + c_2(k_{0z} - k_{1z})(k_{\tau z} + k_{2z})]/[c_1(k_{0z} + k_{2z})(k_{\tau z} + k_{1z}) - c_2(k_{0z} + k_{1z})(k_{\tau z} + k_{2z})]$$

$$B = 2c_1c_2k_{0z}(k_{1z} - k_{2z})/[c_1(k_{0z} + k_{2z})(k_{\tau z} + k_{1z}) - c_2(k_{0z} + k_{1z})(k_{\tau z} + k_{2z})]$$
(10)

$$E_{1} = -2c_{2}k_{0z}(k_{\tau z} + k_{2z})/[c_{1}(k_{0z} + k_{2z})(k_{\tau z} + k_{1z}) - c_{2}(k_{0z} + k_{1z})(k_{\tau z} + k_{2z})]$$

$$E_{2} = 2c_{1}k_{0z}(k_{\tau z} + k_{1z})/[c_{1}(k_{0z} + k_{2z})(k_{\tau z} + k_{1z}) - c_{2}(k_{0z} + k_{1z})(k_{\tau z} + k_{2z})].$$

From (5) and (7) it follows that at $\alpha > k_{0z}^2/k_0^2$ a damping solution appears on both sides of the crystal surface (surface wave). The phase velocity of such a wave is smaller than that of light in vacuum. Owing to this, the Cherenkov mechanism of radiation of a particle, uniformly moving over the crystal surface, is realizable. Damping of waves along the z axis is thus not associated with a crystal self-absorption but is determined by the effect of a total external reflection under diffraction conditions.

Substituting the wavefunctions of the photon from (5) and (8) into (4) taking into account (2), the following expression is obtained for the spectral-angular radiation distribution of an electron, which moves in the time span from $-T_1$ to T_2 and intersects the crystal surface at the time moment t = 0:

$$\frac{\partial^2 N_{\pi}}{\partial \omega \ \partial \Omega} = \frac{e^2 \omega}{4\pi^2 \hbar c^3} \left| \int_{-T_1}^0 \left[(v \cdot e_{\pi}) \left[\exp(iq_0 vt) + A \exp(iq'_0 vt) \right] \right] \right. \\ \left. + (v \cdot e_{\pi\tau}) B \exp(iq_{0\tau} vt) \right] dt + \int_0^{T_2} \sum_{\mu=1,2} \left[(v \cdot e_{\pi}) E_{\mu} \exp(iq_{\mu} vt) \right] \\ \left. + (v \cdot e_{\pi\tau}) E_{\mu} c_{\mu} \exp(iq_{\mu\tau} vt) \right] dt \right|^2$$
(11)

where the pulses transmitted take on the form

$$q_{0} = (\omega - k_{0t} \cdot v_{t})v^{-1} + k_{0z}\theta_{0}$$

$$q'_{0} = (\omega - k_{0t} \cdot v_{t})v^{-1} - k_{0z}\theta_{0}$$

$$q_{0t} = (\omega - k_{tt} \cdot v_{t})v^{-1} - k_{tz}\theta_{0}$$

$$q_{\mu} = (\omega - k_{0t} \cdot v_{t})v^{-1} + k_{\mu z}\theta_{0}$$

$$q_{\mu \tau} = (\omega - k_{tt} \cdot v_{t})v^{-1} + k_{\mu z}\theta_{0}.$$
(12)

At $T_{1,2} \rightarrow \infty$ a non-zero contribution to (11) will be made by terms whose real part of the pulse transmitted may become zero. That is why on integration the terms which correspond solely to the reflected diffracted wave and the transmitted diffracted wave into the medium remain:

$$\partial^2 N_{\pi} / (\partial \omega \,\partial \Omega) = (e^2 \omega / 4\pi^2 v^2 \hbar c^3) (v \cdot e_{\pi\tau})^2 |Bl_{0\tau} - \sum_{\mu=1,2} E_{\mu\tau} l_{\mu\tau}|^2$$
(13)

where the coherent lengths $l_{0\tau} = (q_{0\tau})^{-1}$ and $l_{\mu\tau} = (q_{\mu\tau})^{-1}$.

In the spectral-angular distribution of (13) the first term corresponds to the electron radiation along the path in vacuum as far as crystal surface intersection, and the terms with $E_{\mu x}$ to an electron when moving in the medium.

The maximum value of the coherent length of electron radiation in vacuum as far as the surface, i.e. $|l_{0r}|_{max} = L_{0r} = |\text{Im}(k_{\tau z}\theta_0)|^{-1}$ is determined by the attenuation of the surface wave field, particle energy and incidence angle θ_0 . Close to the exact Bragg condition ($\alpha = 0$), $L_{0r} = c\gamma/\omega\theta_0$, where γ is the Lorentz factor of a relativistic electron. Thus, an electron starts to radiate effectively at a distance from the surface of the order of magnitude $c\gamma/\omega$, i.e. a factor of γ larger than the radiation wavelength. Moreover, the coherent length value $L_{\mu \tau} = |l_{\mu \tau}|_{max}$, corresponding to the radiation of an electron when moving in the medium, is substantially affected by the self-absorption of quanta in a crystal and multiple-scattering phenomenon. The effect of multiple scattering is taken account of with the aid of a mean square angle of multiple scattering per unit of length $\overline{\theta_s^2} = E_s^2/E^2 L_R$ [14], where $E_s = 21 \text{ MeV}$, E is the electron energy and L_R is the radiation length. The coherent lengths of the radiation in the medium are thus determined by the expression

$$L_{\mu\tau} = [\mathrm{Im}(k_{\mu z}\theta_0) + k_{\mu}(\overline{\theta_s^2}/2)L_{\mu\tau}]^{-1}.$$
 (14)

When the incidence angles θ_0 of an electron upon the surface are small, the quantities $L_{\mu\tau}$ are limited first of all to the value of the coherent bremsstrahlung length



Figure 2. Transit of an electron e^- through a crystal with the diamond type structure. The surface is parallel to (001) planes. The electron velocity projection on to the surface makes an angle of 30° with the (100) direction.

 $L_{BS} = (2E/E_R)(L_R c/\omega)^{1/2}$ [15]. With $\theta_0 \rightarrow 0 L_{0r} \ge L_{BS}$ and, in (13), only the first term may be left. Then the angular distribution of SPXR will take the form

$$dN_{\pi}/d\Omega = [e^{2}(v \cdot e_{\pi\tau})^{2}/4\pi\hbar c^{3}v][|B(\omega_{0\tau})|^{2}L_{0\tau}(\omega_{0\tau})\omega_{0\tau}/(1-n_{t}\cdot v/c)]$$
(15)

where $\omega_{0r} = |2\pi\tau \cdot v|(1 - n_t \cdot v/c)^{-1}$. Distribution (15) has a maximum near the double Bragg angle of $\varphi = 2\varphi_{BR} = 30^\circ$, where the value $\alpha \leq |\chi_0|$, i.e. the radiation propagating at a very large angle to the electron velocity. When $\theta_0 = 0$, the vacuum coherent length L_{0r} is restricted to the crystal length L. In this case, expression (15), when L_{0r} is replaced by L, describes the angular distribution of SPXR of an electron moving along the crystal to the vacuum interface and coincides with the expression obtained in [6] for parallel movement of a particle over the surface of space-periodic medium.

It is worth noting that, as an electron moves in the medium, the bremsstrahlung arising can also diffract on the set of planes under consideration. This diffracted bremsstrahlung (DB) manifests itself as an additive to SPXR. Under certain conditions, the DB contribution may be substantial and it should be taken account of.

3. Spectral-angular SPXR characteristics for the diamond-type structure crystals

Consider now the spectral-angular characteristics of radiation from a relativistic electron passing over a single-crystal plate with diamond-type structure (Ge, Si and C). Let a crystal be cut so that its surface is parallel, for example, to the (001) planes. Then three reciprocal lattice vectors turn out to be parallel to the surface, which correspond to the ($\overline{400}$), ($\overline{220}$) and ($\overline{220}$) planes, having a structure factor which is not equal to zero (figure 2).

The angular distribution and lines of constant radiation intensity for one of the Ge crystal reflections are presented in figures 3 and 4, when the electron energy is 500 MeV, and the angle of the incidence upon the surface is $\theta_0 = 10^{-5}$ rad. The angle φ is taken from the direction of the tangent component of an electron velocity vector, and the angle θ is taken with respect to the z axis. The tangent component of the velocity vector makes an angle of 30° with the crystal direction $\langle 100 \rangle$. Diffraction occurs on $(\bar{2}20)$ planes. The distribution has a typical double-peaked form for the parametric radiation mechanism [1] with a dip in the direction of the double Bragg angle of $\varphi = 2\varphi_{BR} = 30^\circ$. Under such conditions the maximum coherent length (as an electron moves in a medium) is limited to a coherent bremsstrahlung length of 2×10^{-2} cm. In this case the vacuum coherent length is 5×10^{-1} cm, i.e. $L_{0r} \ge L_{BS}$ and that is why the main contribution to the

Figure 3. Angular distribution of SPXR for the Ge crystal ($\theta_0 = 10^{-5}$ rad; E = 500 MeV; ($\overline{2}20$) reflection).



Figure 5. The integral number of SPXR quanta in the angle $\Delta \Omega = 10^{-5}$ sr as a function of electron energy for the (220) reflection of a Ge crystal at $\theta_0 = 10^{-5}$ rad.



Figure 4. Constant-intensity lines $dN_x/d\omega$ for Ge $(\theta_0 = 10^{-5} \text{ rad}, E = 500 \text{ MeV}; (\overline{2}20) \text{ reflection}).$



Figure 6. Dependence of radiation coherent length L_{0r} in vacuum and radiation coherent lengths $L_{1,2r}$ in a medium on the incidence angle of an electron with 500 MeV energy on the surface for the ($\overline{2}20$) reflection of a Ge crystal.

distribution is made by a vacuum term. Analysis shows that in this case the DB contribution is much smaller than the SPXR intensity with the electron moving in the medium. So the DB contribution to the general distribution may be ignored.

In figure 5 the number ΔN_{π} of sPXR quanta in the fixed angle $\Delta \Omega = 10^{-5}$ sr is given as a function of the electron energy. Such a quasithreshold nature of radiation is attributed to the fact that radiation conditions are satisfied at any energies and at any $\alpha > 0$. However, the radiation intensity is substantial only in the case when a radiated photon is close to the exact Bragg conditions of $\alpha \approx |\chi_0|$. In our case this is possible at electron energies of more than 50–100 MeV.

Table 1. Basic parameters of SPXR for Ge, Si and C crystals: $\hbar\omega$ is the SPXR quantum energy; $\theta_c = \theta - \pi/2$, angular coordinate of the distribution maximum with respect to θ ; $\Delta\theta$, $\Delta\varphi$, widths of the half-height of one of the SPXR peaks; ΔN_x , total number of quanta in the reflection.

Crystal (hkl)	ħω (keV)	$2\varphi_{BR}$ (deg)	$ \chi_0 \times 10^6$	x ₇ × 10 ⁶	θ, (mrad)	Δθ (mrad)	Δφ (mrad)	$\Delta N_{\pi} \times 10^6$
Ge (400) Ge (220) Ge (220)	5.06 11.85 3.20	120 30 210	84.6 14.8 208.9	24.5 8.3 116.5	8.4 3.1 12.0	5.0 1.2 11.1	12.0 4.5 25.1	1.1 1.9 19.3
Si (220)	12.54	30	7.3	3.5	2.2	1.0	3.4	0.6
C (220)	19.01	30	4.7	1.2	1.9	0.9	3.3	0.13

In figure 6 the dependence of the coherent lengths L_{0r} , L_{1r} and L_{2r} on the incidence angle θ_0 of an electron on the surface is given. As is seen, at small angles of incidence the main contribution to the radiation is made by the vacuum term, and L_{1r} and L_{2r} are restricted to the bremsstrahlung length. At $\theta_0 = 10^{-4}$ rad all the coherent lengths become equal and with a subsequent increase in the angle the main contribution to the SPXR will be made by radiation associated with the electron motion in the medium.

Table 1 gives the main parameters of the spectral-angular distributions of SPXR for some of reflections of Ge, Si and C crystals. Ge has the largest quanta yield at the expense of a higher $|\chi_{\tau}|$ value. The angular width of peaks in φ is determined from the relation $\Delta \varphi \approx (\gamma^{-2} + |\chi_0|)^{1/2}$. The position of the SPXR maximum with respect to θ corresponds to the critical angle of total external reflection under diffraction conditions [6].

4. Conclusion

Special features of the spectral and angular distributions and energy dependence of the quantum yield of SPXR are analogous to the characteristics of PXR generated inside a crystal. At the same time, at sufficiently small incidence angles of an electron on the crystal surface the main contribution to the surface radiation intensity may be made by the vacuum trajectory. In this case, multiple scattering does not affect the radiation process and the vacuum coherent length is limited to the real length of the plane. Let us estimate the possibility of observing SPXR experimentally. Let an electron beam have an energy of 500 MeV, a width of 10^{-1} cm, an angular spread of 10^{-4} rad and an average current of 1 μ A. Then, with a crystal surface length of the order of 1 cm, approximately 0.01% of all particles experience effective radiation. The SPXR yield, for example, for the ($\overline{2}20$) reflection of Ge will be of the order of 10^2 quanta s⁻¹. Sufficiently high spectral and angular densities of the radiation distribution and the possibility of smooth frequency changing when a plate rotates with respect to the electron beam make the SPXR mechanism rather useful in creating a highly intensive x-ray frequency tunable source.

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