Dynamic peaks of transition x-rays emitted during the passage of a charged particle through a single crystal

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(Submitted November 14, 1974)
Zh. Eksp. Teor. Fiz. **68**, 2038–2046 (June 1975)

The dynamic peaks of transition x rays produced in a "thick" single crystal were investigated both in Laue and Bragg cases. A numerical calculation has been carried out of the angular and frequency spectra near the Bragg frequencies for different values of the Lorentz ultrarelativistic charge factor. The formation of the dynamic peaks in crystals of "intermediate" thickness was investigated in the special case of nearly backward reflection.

PACS numbers: 61.80.

It was shown in previous papers[1,2] that when an ultrarelativistic charged particle passes through a single crystal, the usual x-ray transition emission produced at the crystal boundaries, and emitted largely in the forward direction (central spot), is accompanied by the emission of x rays at the Bragg frequencies at Bragg angles (lateral spots). When the crystal is not too thin (see[1] for further details), the central and lateral spots contain narrow high-intensity maxima, the so-called dynamic peaks.

The general formulas obtained in[1] give the angular and frequency spectra for the above radiation. These formulas are very complicated in form, but become much simpler (although they are still relatively complicated) for a "thick" crystal, i.e., when there is substantial absorption of both normally and anomalously (Borrmann effect) transmitted waves.

In this paper, we shall be largely concerned with the latter case, and will carry out analytic integration of the corresponding formulas with respect to the azimuthal angle, both in Laue and Bragg cases. We will then integrate with respect to polar angle and frequency, and this will enable us to calculate the number of quanta emitted into the central and lateral spots for different values of the Lorentz charge factor. Some preliminary results were published in[3] for the Laue case.

To investigate the behavior of the dynamic peaks as a function of thickness, including "intermediate" values, we finally consider the Bragg case for almost backward reflection for which the basic formulas are simpler.

We note that a similar problem was considered in[4]. The preliminary estimates given in these papers were too high, and were subsequently corrected, but no numerical calculations were carried out.

1. BASIC FORMULAS AND INTEGRATION WITH RESPECT TO THE AZIMUTH

As noted in[1], the spectrum of x-ray transition radiation near the Bragg frequencies is a complicated function of the crystal thickness. For the sake of simplicity, therefore, we shall begin by considering a sufficiently thick crystal such that the generated radiation tends to its limiting values. The emission intensities in the central and lateral spots, W and W_h, are then given by Eqs. (I.42) in the Laue case, and by (I.32), (I.33), and (I.45) in the Bragg case.[1)] It will be convenient to introduce the azimuthal and polar angles ϕ and ϑ, where ϕ is measured from the plane containing the direction of motion of the charge $(\mathbf{n})$ and the reciprocal lattice vector $\mathbf{K}_h$ (multiplied by 2π). The angle ϑ is measured from the direction of $\mathbf{n}$ for the central spot, and from the direction of $(\omega/c)\mathbf{n}+\mathbf{K}_h$ for a lateral spot. The quantities $d\mathbf{k}_\perp$ and $d\mathbf{k}_{\perp h}$ in (I.32), (I.33), and (I.42) can then be replaced by $(\omega^2/c^2)\vartheta d\vartheta d\phi$.

We must now integrate W and W_h with respect to the azimuthal angle ϕ. We note that the integrands in the above formulas contain the characteristic denominator

$$|D_\alpha|^2=A\cos^2\phi+B_\alpha\cos\phi+C_\alpha \quad (\alpha=n,\,p), \tag{1}$$

where A, B_α, and C_α can be readily obtained in explicit form from (I.9) and (I.10).

Integration with respect to ϕ can be carried out, for example, with the aid of the theory of residues. We shall use the substitution

$$t=\mathrm{tg}\,(\phi/2) \tag{2}$$

and then consider the resulting integrals in the complex plane of t. As ϕ varies from zero to 2π, the variable t runs along the real axis. The integrals can be found in terms of residues at poles in the upper half-plane. This yields very complicated expressions which we shall not reproduce here.

However, integration with respect to ϕ can be carried out very simply with adequate accuracy if we use certain physical ideas and introduce the corresponding approximations in the initial formulas.

As noted in[1], well away from a dynamic peak due to a minimum of the quantity given by (1), the central-spot intensity is the same as the intensity of the usual transition emission described by the macroscopic theory, whereas the lateral-spot intensity is very low. Consequently, it is interesting to calculate the difference between the central-spot intensity (number of photons) and the lateral-spot intensity (number of photons) near the dynamic peaks.

The quantity given by (1) has a minimum for

$$\cos\phi=-B_\alpha/2A. \tag{3}$$

When

$$|B_\alpha|\leqslant 2A, \tag{4}$$

the dynamic peak is obtained for physical values of ϕ, i.e., real ϕ. Elsewhere, the dynamic peak is absent. We shall evaluate the integrals of W and W_h only for those cases where (4) is satisfied.

Using (I.32), (I.33), or (I.42), we find that the integrals have the general form

$$I=\int_0^{2\pi}\frac{F(\cos\phi)\,d\phi}{A\cos^2\phi+B_\alpha\cos\phi+C_\alpha}=2\int_0^{\pi}\frac{F(\cos\phi)\,d\phi}{A\cos^2\phi+B_\alpha\cos\phi+C_\alpha},\tag{5}$$

where $F(\cos\phi)$ is a certain function of $\cos\phi$, which has no singularities for physical values of ϕ.

Expanding the denominator in the integrand in (5) around the minimum point, we obtain

$$A\cos^2\phi+B_\alpha\cos\phi+C_\alpha=\frac{P_\alpha^2}{4A}+\frac{4A^2-B_\alpha^2}{4A}(\phi-\phi_0)^2\tag{6}$$

where ϕ_0 is a solution of (3) between 0 and π, and

$$P_\alpha=(4AC_\alpha-B_\alpha^2)^{1/2}.\tag{7}$$

Substituting (6) in (5), taking out the value of F for $\phi=\phi_0$, and integrating with respect to ϕ, we obtain

$$I=\frac{8\pi A}{P_\alpha(4A^2-B_\alpha^2)^{1/2}}F\left(-\frac{B_\alpha}{2A}\right).\tag{8}$$

It is clear from this formula that as $4A^2-B_\alpha^2\to 0$, the quantity I increases without limit. However, this is connected with the expansion given by (6) which is not entirely correct in this case. When $4A^2-B_\alpha^2=0$, the expansion takes the form

$$A\cos^2\phi+B_\alpha\cos\phi+C_\alpha=\frac{P_\alpha}{4A}+\frac{A}{4}(\phi-\phi_0)^4.\tag{9}$$

Therefore, instead of (8) we have

$$I=\frac{2\pi\sqrt{2A}}{P_\alpha^{3/2}}F\left(-\frac{B_\alpha}{2A}\right).\tag{10}$$

It is clear that the exact formula for the integral I must approach asymptotically the expressions given by (8) and (10) for large and small values of $4A^2-B_\alpha^2$, respectively.

We must now establish the range of validity of these formulas. We note that, when $4A^2-B_\alpha^2=8AP_\alpha$, the two formulas are identical. This means that (8) is valid for

$$4A^2-B_\alpha^2\gg 8AP_\alpha,\tag{11}$$

and (10) is valid when the reverse inequality is satisfied. We also note that, if the correct expressions for A, B_α, and P_α are taken into account, condition (11) can also be written in the form

$$A-C_\alpha\gg 2P_\alpha.\tag{12}$$

Using (8) and (10), we can readily calculate the contribution of the dynamic peak to the number of photons in the central and lateral spots.

2. LAUE CASE

We shall determine the number of photons in the central and lateral spots, N and N_h, which we shall write in the form

$$N=\int[N_{tr}(\nu,\vartheta)+N'(\nu,\vartheta)]\,d\nu\,d\vartheta,$$
$$N_h=\int N_h(\nu,\vartheta)\,d\nu\,d\vartheta,\tag{13}$$

where

$$N_{tr}(\nu,\vartheta)=2|g_{00}|^2\vartheta^3/137\pi\eta_0^2\eta^2\tag{14}$$

determines the spectrum of the usual transition emission given by the macroscopic theory (the notation is the same as in[1] except that, for the sake of simplicity, we have omitted the symbol ~). Moreover,

$$N'(\nu,\vartheta)=\int_0^{2\pi}N(\nu,\vartheta,\phi)\,d\phi-N_{tr}(\nu,\vartheta),$$

$$N_h(\nu,\vartheta)=\int_0^{2\pi}N_h(\nu,\vartheta,\phi)\,d\phi.\tag{15}$$

Using (8), and assuming that (11) is satisfied, we have

$$N'(\nu,\vartheta)=\frac{2|g_{0h}|^4\vartheta^2}{137\pi\eta\sin 2\theta_B}\left[\frac{(A-C_n)^{1/2}}{\eta^2P_n}+\frac{G^2\cos^2 2\theta_B}{P_p(A-C_p)^{1/2}}\right],$$
$$N_h(\nu,\vartheta)=\frac{2|g_{0h}|^2\vartheta^2\,\mathrm{ctg}\,2\theta_B}{137\pi}\left[\frac{(A-C_n)^{1/2}}{\eta P_n}+\frac{\eta G^2}{P_p(A-C_p)^{1/2}}\right],\tag{16}$$

where θ_B is the Bragg reflection angle and

$$G=2\eta-\cos 2\theta_B[2g'\sin^2\theta_B+\vartheta^2+(1-\beta^2)\cos 2\theta_B+4\nu\sin^2\theta_B+|g_{0h}|^2\cos^2 2\theta_B/\eta].\tag{17}$$

When the condition

$$4A^2-B_p^2\ll 8AP_p,\tag{18}$$

is satisfied, the principal parts of $N'(\nu,\vartheta)$ and $N_h(\nu,\vartheta)$ are given by the following formulas if we use (10):

$$N'(\nu,\vartheta)=2^{1/2}|g_{0h}|^4\vartheta^2G^2\cos^2 2\theta_B/137\pi\eta P_p^{3/2}\sin 2\theta_B,$$
$$N_h(\nu,\vartheta)=2^{1/2}|g_{0h}|^2\vartheta^2\eta G^2\,\mathrm{ctg}\,2\theta_B/137\pi P_p^{3/2}.\tag{19}$$

On the other hand, when a condition analogous to (18) is satisfied, but with p replaced by n, the presence of the factor $\sin\phi$ ensures that the corresponding contribution to the dynamic peak is small according to (10).

The integration with respect to ϑ and ν in (13) cannot be carried out analytically. We note, however, that, for sufficiently large $|\nu|$, integration with respect to ϑ can be carried out explicitly with adequate accuracy. In fact, suppose that

$$|\nu|\gg 1-\beta^2,\ |g'|,\ |g_{0h}|,\ |g_{h0}|.\tag{20}$$

We can then show that

$$B_\alpha\approx-16\vartheta\eta^2\nu\sin 2\theta_B\sin^2\theta_B,$$

and condition (4) reduces to the following simple inequality:

$$\vartheta\geqslant\vartheta_0,\tag{21}$$

where $\vartheta_0=|\nu\tan\theta_B|$.

Now suppose that an inequality analogous to (20) is satisfied, with $|\nu|$ on the left-hand side replaced with ϑ^2. The expressions given by (16) can then be rewritten in the form

$$N'(\nu,\vartheta)=\frac{|g_{0h}|^4}{137\pi g''\vartheta^7\sin 2\theta_B}\left\{(\vartheta^2-\vartheta_0^2)^{1/2}+\frac{\vartheta_0^2\cos^4 2\theta_B}{(\vartheta^2-\vartheta_0^2)^{1/2}}\right\}$$
$$N_h(\nu,\vartheta)=\frac{|g_{0h}|^2\,\mathrm{ctg}\,2\theta_B}{137\pi g''\vartheta^3}\left\{(\vartheta^2-\vartheta_0^2)^{1/2}+\frac{\vartheta_0^2\cos^2 2\theta_B}{(\vartheta^2-\vartheta_0^2)^{1/2}}\right\}.\tag{22}$$

Using these formulas, we can readily evaluate the integrals

$$N'(\nu)=\int N'(\nu,\vartheta)\,d\vartheta,\qquad N_h(\nu)=\int N_h(\nu,\vartheta)\,d\vartheta.\tag{23}$$

For large $|\nu|$, we obtain

$$N'(\nu)=\frac{|g_{0h}|^4(1+5\cos^4 2\theta_B)}{32\cdot 137g''\vartheta_0^5\sin 2\theta_B},\tag{24}$$

and

$$N_h(\nu)=\frac{|g_{0h}|^2\,\mathrm{ctg}\,2\theta_B}{4\cdot 137g''\vartheta_0}(1+\cos^2 2\theta_B).$$

We note that the expressions for $N'(\nu)$ and $N_h(\nu)$ depend on ϑ_0, i.e., on $|\nu|$, in different ways. However, it is important to recall that the above formulas are valid only for $|\nu|\ll 1$. For larger values of $|\nu|$, the angle ϑ_0 becomes large. When this angle approaches $\pi/2$, the dynamic peaks will, of course, vanish altogether. We can therefore use (4) to find the limiting values (ν_1 and ν_2) such that, when ν lies outside the interval (ν_1, ν_2), we have $N'(\nu) = N_h(\nu) = 0$. It follows that integration of these functions with respect to ν may be carried out only between ν_1 and ν_2.

As an illustration, we have calculated the number of photons in the central and lateral spots near the dynamic peaks for different values of the Lorentz charge factor γ. The calculation was performed for single crystals of LiH which has cubic NaCl-type structure with lattice constant equal to 4.08 Å. The charge was allowed to travel along the [111] axis and the reflection occurred on ($00\bar{2}$) planes, i.e., the reflection angle was $\theta_B = 35°15'$. The corresponding frequency was $\omega_B = 5.268$ keV. The relative uncertainty in the numerical calculation did not exceed 0.5%.

Figure 1 shows the functions $N'(\nu, \vartheta)$ and $N_h(\nu, \vartheta)$ for different values of ν. They were calculated from (16) or (19), depending on whether (11) or (18) was satisfied. The broken curve corresponds to $N_{tr}(\nu, \vartheta)$, calculated from (14).

It is clear that curves 2–6 have a valley in the region of small ϑ. This is connected with the fact that (4) is not satisfied for small ϑ. The angle for which $|B_\alpha| = 2A$ ($\alpha = p$ or $\alpha = n$) will be denoted by ϑ_α.

Figure 2 shows graphs of $N'(\nu)$ and $N_h(\nu)$ for different values of the Lorentz factor. It is clear from the figure that $N_h(\nu)$ is greater than $N'(\nu)$ by roughly an order of magnitude. The broken curve shows the corresponding quantity for the central spot (with $\gamma = 1000$)

$$N(\nu) = \int [N_{tr}(\nu, \vartheta) + N'(\nu, \vartheta)]\, d\vartheta. \tag{25}$$

As can be seen, for $\nu = 0$, the quantity $N_h(\nu)$ amounts to about 63% of $N(\nu)$.

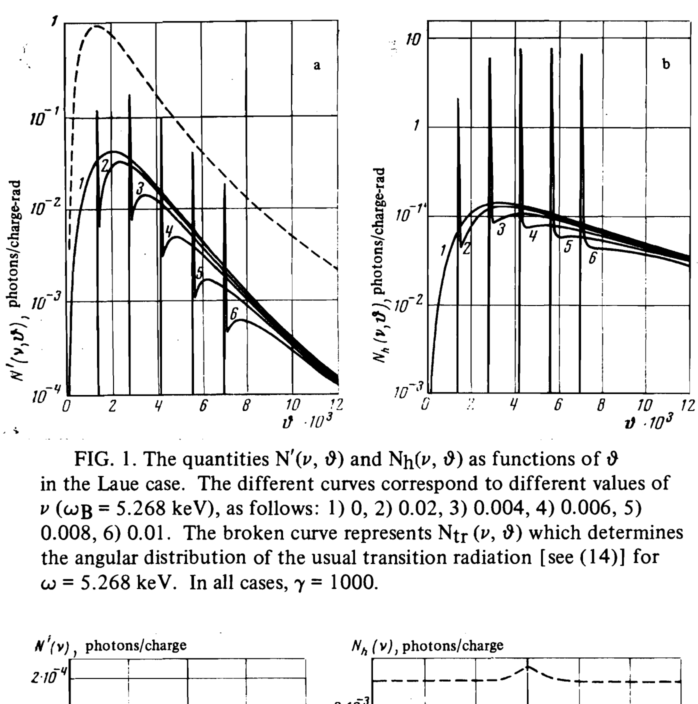

FIG. 1. The quantities $N'(\nu, \vartheta)$ and $N_h(\nu, \vartheta)$ as functions of ϑ in the Laue case. The different curves correspond to different values of ν ($\omega_B = 5.268$ keV), as follows: 1) 0, 2) 0.02, 3) 0.004, 4) 0.006, 5) 0.008, 6) 0.01. The broken curve represents $N_{tr}(\nu, \vartheta)$ which determines the angular distribution of the usual transition radiation [see (14)] for $\omega = 5.268$ keV. In all cases, $\gamma = 1000$.

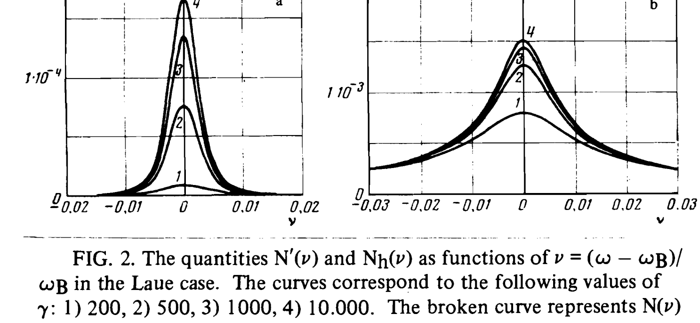

FIG. 2. The quantities $N'(\nu)$ and $N_h(\nu)$ as functions of $\nu = (\omega - \omega_B)/\omega_B$ in the Laue case. The curves correspond to the following values of γ: 1) 200, 2) 500, 3) 1000, 4) 10.000. The broken curve represents $N(\nu)$ [see (25)] for $\gamma = 1000$, $\omega_B = 5.268$ keV.

3. BRAGG CASE

As noted in[1], the dynamic peak is absent from the central spot in the Bragg case. Insofar as the lateral spot is concerned, the number of photons in it is negligible by analogy with the Laue case, considered in the preceding section, when $\vartheta < \vartheta_\alpha$ and (4) is not satisfied. Near ϑ_p, when $|A - C_p| \ll 2P_p$, we can use (10) to show that the number of photons is given by

$$N_h = \int N_h(\nu, \vartheta)\, d\nu\, d\vartheta,$$

$$N_h(\nu, \vartheta) = \frac{\sqrt{2}\, |g_h|^2 \vartheta^2 G^2 \operatorname{ctg} 2\theta_B}{137\pi\eta P_p^{3/2}} \left(\eta + \frac{|g_h|^2 \cos 2\theta_B}{\eta}\right)^2. \tag{26}$$

For sufficiently large ϑ, such that $A - C_\alpha \gg 2P_\alpha$, we have from (8)

$$N_h(\nu, \vartheta) = \frac{2|g_h|^2 \vartheta^2 \operatorname{ctg} 2\theta_B}{137\pi\eta} \left\{ \frac{(A - C_n)^{1/2}}{P_n} \left(1 + \frac{|g_h|^2}{\eta^2 \cos 2\theta_B}\right)^2 + \frac{G^2}{P_p (A - C_p)^{1/2}} \left(\eta + \frac{|g_h|^2 \cos 2\theta_B}{\eta}\right)^2 \right\}, \tag{27}$$

where G is given by (17).

Equations (26) and (27) refer to the case where the angle $2\theta_B$ is very different from π. When $2\theta_B$ approaches π, the condition given by (4) can be satisfied only for a small range of values of ϑ. Moreover, it is clear from the expression for B_α that, when $\nu < 0$, this interval may not exist. Since the values of A and C_α are then small, only those cases for which $|A - C_\alpha| \ll P_\alpha$ will largely be realized. This means that the contribution of the normal polarization ($\alpha = n$) will be substantially reduced. In the limit, when $2\theta_B = \pi$, we obtain the expressions given by (I.29), for which the normal polarization is entirely absent.

Numerical calculations performed for the case where the charge was allowed to travel along the [111] axis and reflection took place on ($\bar{2}0\bar{2}$) planes showed that the form of the curves representing $N_h(\nu, \vartheta)$ as a function of ϑ and $N_h(\nu)$ as a function of ν is very similar to the corresponding results for the lateral spot in the Laue case (Fig. 1b, 2).

Figure 3 shows graphs of N' and N_h in the Laue case and N_h in the Bragg case as functions of γ. For comparison, the latter calculations were performed for two values of ω_B. We note that for sufficiently large values of γ, such that $\gamma^{-2} \ll |g'|$, the quantity N_h reaches a constant value.

4. NEARLY BACKWARD REFLECTION

We have, so far, confined our attention to sufficiently thick crystals for which (I.40) was satisfied. To investigate the dynamic peak for arbitrary thickness (small, intermediate, and large), we shall now consider Bragg reflections in nearly backward directions ($2\theta_B = \pi$) when the basic formulas are relatively less complicated.

For an arbitrary thickness, the number of photons in the central and lateral spots is given by

$$N=\frac{\omega^2\vartheta}{(2\pi)^6\hbar c}\int|E^{\mathrm{vac}}|^2\,d\nu\,d\vartheta\,d\phi,\quad N_h=\frac{\omega^2\vartheta}{(2\pi)^6\hbar c}\int|E_h^{\mathrm{vac}}|^2\,d\nu\,d\vartheta\,d\phi, \tag{28}$$

where the integrands are given by equations (17) and (18) in[5]. We have used these formulas in a numerical calculation for a single crystal of diamond (lattice constant 3.56 Å) with the charge allowed to travel along the principal axis. We considered the emission in the region of the Bragg frequency $\omega_B = 5.22$ keV, corresponding to nearly backward reflection. Numerical calculations of the angular distribution showed that the dynamic peaks appear only for sufficiently large values of the crystal thickness when condition (I.34) is not satisfied. Insofar as the angular width of the dynamic peak is concerned, it is found that, for intermediate thicknesses, this width is inversely proportional to the thickness and, for large thicknesses, it ceases to be a function of thickness and is determined exclusively by absorption (see also[5,6]).

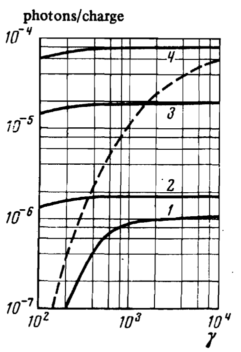

FIG. 3

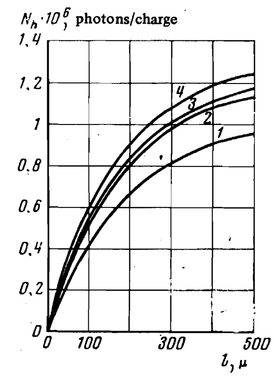

FIG. 4

FIG. 3. Total number of photons in the central and lateral spots as a function of γ. Curve 1 gives N′ (Laue case, $\omega_B = 5.268$ keV), 2—N_h (Bragg case, $\omega_B = 3.226$ keV), 3—N_h (Bragg case, $\omega_B = 5.268$ keV), 4—N_h (Laue case, $\omega_B = 5.268$ keV). Broken curve shows $N_{tr} = \int N_{tr}(\nu, \vartheta)\,d\vartheta d\nu$ for $\Delta\nu = 0.005$, $\omega_B = 5.268$ keV or $\Delta\omega = 26.3$ eV.

FIG. 4. Total number of photons N_h reflected almost exactly in the backward direction as a function of the thickness of the crystal plate. The various curves correspond to the following values of γ: 1) 200; 2) 500; 3) 1000; 4) 10.000; $\omega_B = 5.221$ keV.

Numerical calculations have also shown that the backward-reflected emission peak corresponds to a valley in the forward-emitted intensity. This distinguishes the Bragg case from the Laue case for which maxima in lateral spots correspond to maxima in central spots (Fig. 2).

Figure 4 shows the number of photons N_h as a function of the crystal thickness l for different values of γ. It is clear that the number of photons reflected in the backward direction tends to saturate as the crystal thickness increases, and gradually increases with increasing Lorentz factor.

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1)References to formulas in [1] will be designated I.

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Translated by S. Chomet
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