Coherent bremsstrahlung on a deformed graphene sheet

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Abstract. We investigate coherent bremsstrahlung by electrons in a periodically deformed two-dimensional crystal. The formula for the corresponding spectral-angular density of the cross-section is derived for an arbitrary deformation field. Applications are given for a graphene sheet.

1. Introduction

The bremsstrahlung of high-energy electrons in crystals is one of the most effective methods for producing quasimonochromatic gamma-quanta. It has been extensively investigated either theoretically and experimentally over the last decade (see, for instance, Refs. [1]-[4]). The corresponding radiation has a number of remarkable properties and has found many important applications. Among them is the generation of intense positron beams. The basic source to creating positrons for high-energy electron-positron colliders is the electron-positron pair creation by hard bremsstrahlung photons produced when a powerful electron beam hits an amorphous target. One possible approach to increase the positron production efficiency is to use a crystal target as a positron emitter. When the crystal axis is aligned with the direction of the incident beam, intense photons are emitted through the coherent bremsstrahlung process and the channeling radiation process. These photons are then converted to electron-positron pairs.

From the point of view of controlling the parameters of the coherent bremsstrahlung it is of interest to investigate the influence of external fields, such as acoustic waves, a temperature gradient, etc., on corresponding characteristics. In Refs. [5, 6] it has been shown that the periodical deformations induced in a crystal by hypersonic waves can either enhance or reduce the bremsstrahlung cross-section (for the influence of the hypersonic waves on the coherent electron-positron pair production in crystals see [7, 8]). In the present paper we investigate the coherent bremsstrahlung by relativistic electrons on a two-dimensional deformed crystal. The general case of the profile function for the deformation will be discussed. As an application, we specify the general formula for the cross-section for the case of graphene sheet.

2. Cross-section of the bremsstrahlung on a two-dimensional deformed crystal

We start our consideration by the bremsstrahlung of electrons on a two-dimensional deformed crystal with a complex unit cell. We assume that the undeformed crystal is flat and coincides with the \((y, z)\)-plane of the cartesian coordinate system \((x, y, z)\). The momentum and
the energy of the radiated photon will be denoted by $k$ and $\omega$, respectively (throughout the paper we use the units with $\hbar = c = 1$). The atoms in the unit cell will be specified by the superscript $j$ and $u^{(j)}_q$ is the Fourier transform of the corresponding potential. Let us denote by $d\sigma^{(j)}_0 = |u^{(j)}_q|^2 \sigma_0(q)d\theta_\gamma d\omega dq$ the cross-section of the bremsstrahlung on an isolated $j$th atom as a function of the transfer momentum $q = p_1 - p_2 - k$, with $p_1$ and $p_2$ being the momenta for the electron in the initial and final states, $\theta_\gamma$ is the angle between the vectors $p_1$, $k$, and the factor $\sigma_0(q)$ does not depend on the type of the atom. For the transferred momenta $q \ll m_e$, with $m_e$ being the electron mass, one has [9]

$$\sigma_0(q) = \frac{e^2 q^2_\perp}{8\pi^2 E_1^2 q^2_\parallel} \left[ 1 + \frac{\omega^2}{2E_1 E_2} - 4y^2(q) \frac{\delta}{q_\parallel} \left( 1 - \frac{\delta}{q_\parallel} \right) \right] \frac{dy(q)/d\theta_\gamma}{\sqrt{1 - y^2(q)}},$$

(1)

where $\delta = 1/l_c$ is the minimum longitudinal momentum transfer and the function $y(\theta_\gamma)$ is given by the relation

$$y(q) = \frac{m_e}{2q_\perp h(q)} \left[ \left( \frac{E_1 \theta_\gamma}{m_e} \right)^2 - h^2(q) - q^2_\perp/m_e^2 \right],$$

(2)

with the notation

$$h(q) = \left( \frac{q_\parallel}{\delta} - 1 - \frac{q^2_\perp}{2E_1 \delta} \right)^{\frac{1}{2}}.$$  

(3)

In (1), $e$ is the electron charge, $E_1$ is the energy of the initial electron, $q_\parallel$ and $q_\perp$ are the parallel and perpendicular components of the transferred momentum with respect to $p_1$. For the formation length of the bremsstrahlung we have the expression $l_c = 2E_1 E_2/(\omega m_e^2)$, where $E_2$ is the energy of the electron after the radiation. The allowed values of the variables are restricted by the conditions

$$q_\parallel \geq \delta + \frac{q^2_\perp}{2E_1}, \quad q_\perp \geq 0, \quad -1 \leq y(q) \leq 1.$$  

(4)

Now the differential cross-section per atom in a two-dimensional crystal with the atoms located at $r = r^{(j)}_n$ is written in the form

$$d\sigma = \sigma(q) d\omega d\theta_\gamma dq = \frac{1}{N_0} \left| \sum_{n,j} u_q^{(j)} e^{-iqr} \right|^2 \sigma_0(q) d\omega d\theta_\gamma dq,$$

(5)

where $N_0$ is the number of atoms in the crystal and the index $n$ enumerates the elementary cells. In a way similar to that for a 3-dimensional crystal, after averaging over the thermal fluctuations, the cross-section is presented in the form

$$\sigma(q) = \frac{1}{N_0} \left[ N \sum_j \left| u_q^{(j)} \right|^2 \left( 1 - e^{-q^2 \overline{u^{(j)}_q}^2} \right) + |U_q|^2 \right] \sigma_0(q),$$

(6)

where $N$ is the number of the elementary cells, $\overline{u^{(j)}_q}^2$ is the temperature-dependent mean-squared amplitude of the thermal vibrations for the $j$th atom. In (6) we have introduced the notation

$$U_q = \sum_{n,j} u_q^{(j)} e^{iqr} e^{-\frac{1}{2} q^2 \overline{u_q^{(j)}}^2},$$

(7)
where \( r_{n0}^{(j)} \) determines the equilibrium positions of the atoms in deformed crystal and \( e^{-\frac{1}{2} f^2 u_{ij}^{(j)}} \) is the Debye-Waller factor.

The part in the cross-section with the first term in the square brackets of (6) does not depend on the orientation of the crystal axis with respect to the momentum of the electron and corresponds to the incoherent effects. The coherent effects are described by the part

\[
\sigma_c (q) = \frac{1}{N_0} |U_q|^2 \sigma_0 (q). \tag{8}
\]

For a deformed crystal the vectors determining the positions of the atoms are presented in the form \( r_{n0}^{(j)} = r_{ne}^{(j)} + u_{n}^{(j)} \), where \( r_{ne}^{(j)} \) corresponds to the equilibrium position in the undeformed crystal and \( u_{n}^{(j)} \) is the atom displacement induced by the deformation. We assume that the undeformed two-dimensional crystal is planar and, hence, the vector \( r_{ne}^{(j)} \) determines the points on the \((y, z)\)-plane. We will consider periodic deformation fields of the form

\[
u_n^{(j)} = u_0 f(k_s r_{ne}^{(j)}), \tag{9}\]

where \( f(x) \) is a periodic function with the period equal \( 2\pi \) and \( \max |f(x)| = 1 \), \( u_0 \) is the amplitude of the deformation. For the vector \( k_s \) one has \( k_s = (0, k_{sy}, k_{sz}) \) and \( k_s = |k_s| = 2\pi/\lambda_s \) with \( \lambda_s \) being the period of the deformation.

The coordinates of the atoms can be presented in the form \( r_{ne}^{(j)} = R_\sigma + \rho^{(j)} \), where \( R_\sigma \) corresponds to the positions of the atoms of one of the primitive lattices, and \( \rho^{(j)} \) are the equilibrium positions for the other atoms inside \( n \)th elementary cell with respect to \( R_\sigma \). For an infinite two-dimensional crystal one has

\[
\sum_{m=-\infty}^{+\infty} F_m(q) = \int_{-\pi}^{+\pi} e^{iyf(x)} dx. \tag{12}\]

For a deformed two-dimensional crystal one has

\[
\sum_{m=-\infty}^{+\infty} e^{i(q+mk_s)R_m} = \frac{(2\pi)^2}{\Delta} \sum_{g} \delta(q \parallel - g_m), \tag{13}\]

where \( q \parallel = (q_y, q_z) \) is the component of the vector \( q \parallel \) parallel to the \((y, z)\)-plane (undeformed crystal), \( \Delta \) is the surface area of the unit cell, \( g = (g_y, g_z) \) is the reciprocal lattice vector and

\[
g_m = g - mk_s. \tag{14}\]

In this case the coherent part of the cross-section is written in the form

\[
\sigma_c (q) = \frac{N}{N_0} \frac{(2\pi)^2}{\Delta} \sum_{m=-\infty}^{+\infty} |F_m(q) u_0| \sum_{g} \delta(q \parallel - g_m) \sigma_0 (q). \tag{15}\]
Substituting this into \(d\sigma_c = \sigma_c(q) \, d\omega d\theta, dq\), after the integration over the components of the transferred momentum parallel to the undeformed sheet we get

\[
d\sigma_c = \frac{e^2 N}{2\pi^2 N_0 E_1^2} \sum_{m, \mathbf{g}} |F_m(q_m u_0)|^2 \frac{|S(q_m, q)|^2}{\sqrt{1 - y^2(q_m)}} q_{m\perp}^2 \rho_m^2 \\
\times \left[ 1 + \frac{\omega^2}{2E_1 E_2} - 4y^2(q_m) \frac{\delta}{q_{m\parallel}} \left( 1 - \frac{\delta}{q_{m\parallel}} \right) \right] \, d\omega dq_x dy(q_m),
\]

(16)

where

\[
q = (q_x, q_y, q_z), \quad q_m = (q_x, g_{m_y}, g_{m_z}),
\]

(17)

and the summation goes under the conditions

\[
q_{m\parallel} \geq \delta + \frac{q_{m\perp}^2}{2E_1}, \quad -1 \leq y(q_m) \leq 1.
\]

(18)

The momentum conservation is written as \(q_S = p_1 - p_2 - k\).

For a flat crystal, when the deformation is absent one has \(F_m(q_m u_0) = F_m(0) = \delta_{m0}\) and the general formula is reduced to

\[
d\sigma_c = \frac{e^2 N}{2\pi^2 N_0 E_1^2} \sum_{\mathbf{g}} |S(q, q)|^2 \frac{q_{m\perp}^2}{\sqrt{1 - y^2(q)}} q_{m\parallel}^2 \\
\times \left[ 1 + \frac{\omega^2}{2E_1 E_2} - 4y^2(q) \frac{\delta}{q_{m\parallel}} \left( 1 - \frac{\delta}{q_{m\parallel}} \right) \right] \, d\omega dq_x dy(q),
\]

(19)

with \(q = (q_x, q_y, q_z)\). The corresponding constraints are obtained from (18) taking \(m = 0\). As is seen, the periodic deformation leads to an additional summation over \(m\) in the expression for the coherent bremsstrahlung cross-section. This corresponds to the generation of a superlattice with the period \(\lambda_x\). The separate terms in the summation over \(m\) are weighted by the factor \(|F_m(q_m u_0)|^2\) which is determined by the profile function of the deformation. In particular, for the sinusoidal deformation field \(f(x) = \sin(x + \varphi_0)\) we have

\[
F_m(y) = e^{im\varphi_0} F_m(y).
\]

(20)

From (16), integrating over \(y\) and \(q_x\), for the spectral dependence of the cross-section we obtain

\[
\frac{d\sigma_c}{d\omega} = \frac{e^2 N}{2\pi^2 N_0 E_1^2} \sum_{\mathbf{g}, m} \int dq_x |F_m(q_m u_0)|^2 |S(q_m, q)|^2 \\
\times q_{m\perp}^2 \left[ 1 + \frac{\omega^2}{2E_1 E_2} - 2\frac{\delta}{q_{m\parallel}} \left( 1 - \frac{\delta}{q_{m\parallel}} \right) \right],
\]

(21)

with the constraint \(q_{m\parallel} \geq \delta + q_{m\perp}^2/(2E_1)\). Note that one has \(q_{m\perp}^2/(2E_1) = (E_2/\omega)(q_{m\perp}/m_e)^2\) and, hence, for the photons with the energies \(\omega > E_2(q_{m\perp}/m_e)^2\) the second term in the righthand side of this constraint is subdominant. We recall that our consideration is valid under the condition \(q_{m\perp}/m_e \ll 1\). For a simple crystal and for the exponential screening of the atomic potential, ignoring the thermal effects, one has

\[
|S(q_m, q)|^2 = |u_{q_m}|^2 = \frac{16\pi^2 Z^2 e^4}{(q_m^2 + R^2)^2},
\]

(22)

with \(R\) being the screening radius and \(Z\) is the number of electrons in an atom.
3. Special cases and applications to graphene

Let us denote by $\theta_e$ and $\alpha_e$ the spherical angles for the vector $p_1$ in the coordinate system connected with the undeformed crystal:

$$p_1 = p_1(\cos \theta_e, \sin \theta_e \cos \alpha_e, \sin \theta_e \sin \alpha_e).$$

(23)

Here $\theta_e$ is the angle between the vector $p_1$ and $x$-axis and $\alpha_e$ is the angle between the projection of the vector $p_1$ on the $(y, z)$ plane and $y$-axis. Then one gets

$$q_m = q_e \cos \theta_e + g_m^{(y)},$$

$$q_m^2 = q_e^2 + g_m^2 + g_{mz}^2 - q_m^2,$$

(24)

with

$$g_m^{(y)} = \sin \theta_e \cos \alpha_e + g_{mz} \sin \alpha_e.$$

(25)

For fixed $m$ and $g$, the condition $q_m \geq \delta + q_m^2/(2E_1)$ determines the limits of the integration over $q_z$ in (21). The formulas (19) and (21), in combination with (24) and (25), give the dependence of the cross-section on the angles $\theta_e$ and $\alpha_e$. The coherence effects induced by the crystal are important when the electron moves close to the crystal plane that corresponds to the angles $\theta_e$ close to $\pi/2$. Relatively simple results are obtained for the motion parallel to the undeformed crystal, $\theta_e = \pi/2$. In this case, one has $q_m = q_m^{(y)} = g_m \cos \alpha_e + g_{mz} \sin \alpha_e$ and $q_m$ does not depend on $q_z$.

Let us specify the general results, given in the previous section, for the case of a graphene sheet. Graphene is a carbon monolayer with honeycomb lattice having the interatomic distance $a = 0.142$ nm. The unit cell contains two atoms each of which generates a triangular sublattice (see figure 1). To have an orthogonal lattice, as an elementary cell we take the one containing four atoms of carbon (see figure 1). For the radius-vectors $\rho^{(j)} = (\rho_y^{(j)}, \rho_z^{(j)})$ of these atoms one has

$$\rho^{(0)} = (0, 0), \quad \rho^{(1)} = \frac{a}{2} \left( -1, \sqrt{3} \right),$$

$$\rho^{(2)} = \frac{a}{2} \left( 3, \sqrt{3} \right), \quad \rho^{(3)} = (a, 0).$$

(26)

For the corresponding reciprocal lattice vector one has

$$g = (g_y, g_z) = \frac{2\pi}{3a} \left( n_y, \sqrt{3}n_z \right),$$

(27)

with $n_y, n_z = 0, 1, 2, \ldots$. For graphene one has one sort of atoms and, hence,

$$S(q_m, q) = u_{q_m} e^{-\frac{1}{2}q_m^2n_z^2} \sum_j e^{iq \cdot \rho^{(j)}}.$$

(28)

Now, by taking into account that the vectors $\rho^{(j)}$ lie in the $(y, z)$-plane and, hence, $q \cdot \rho^{(j)} = g \cdot \rho^{(j)}$, for an elementary cell under consideration one gets

$$\sum_j e^{iq \cdot \rho^{(j)}} = 4 \left[ 1 + (-1)^{n_y+z} \left[ 1 + (-1)^{n_y} \cos(\pi n_z/3) \right]\right].$$

(29)

In addition, one has $N/N_0 = 1/4$. 


4. Conclusion
We have investigated the coherent bremsstrahlung of electrons on a deformed two-dimensional crystal with a complex base. For the deformation field we have considered general profile function. The cross-section for the spectral-angular distribution of the radiated photons is given by the expression (16), where the function $y(q)$ is related to the angle $\theta_\gamma$ between the momentum of the initial electron and the wave vector of the photon by (2). In a special case, when the deformation is absent we obtain the cross-section on a flat crystal. In the presence of periodical deformation, the expression for the cross-section contains an additional summation over the reciprocal lattice vector of the corresponding one dimensional superlattice. After the integration over the angle $\theta_\gamma$, we obtain the spectral density of the cross-section, given by the expression (21). The general results are specified for the graphene sheet. The numerical analysis of the cross-section is in progress and will be presented elsewhere.

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