Bremsstrahlung of fast electron on graphene

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Abstract. Polarization Bremsstrahlung (PB) [1] and Static (ordinary) Bremsstrahlung (SB) [2] of fast electron scattered on graphene are investigated theoretically for relativistic and non-relativistic projectile velocities. In the framework of the first Born approximation spectral, angular and velocity dependences of PB and SB are calculated and analyzed for various incident electron angles. Coherent and incoherent interactions between electron and two-dimensional graphene are taken into account in the calculations.

1. Introduction
Why graphene? First of all, it is a perfect two-dimensional crystal where a transmitted momentum is discrete in the plane and is arbitrary across it. What can it give in bremsstrahlung processes? How will it be manifested in coherent and incoherent channels? Finally, active work is now underway on obtaining large-size loose-hanging, self-supporting graphene films, which allows looking forward to the performance of an experiment [3].

2. General expression for cross-section of process on ensemble of atoms
The cross-section of a photo process on an ensemble of target atoms looks like (in case of a monatomic target)

\[ d\sigma_{\text{target}} = \left| \sum_{i} \exp\left(i\mathbf{q} \cdot \mathbf{r}_i\right) \right|^2 d\sigma_{\text{atom}}, \]  

where the sum is over all target atoms being in the volume of interaction, \( d\sigma_{\text{atom}} \) is the differential cross-section of the process on one atom under consideration, \( \mathbf{q} = (\mathbf{p}_f - \mathbf{p}_i)/\hbar - \mathbf{k} \) is the wave vector transferred from an incoming electron to the target, \( \mathbf{p}_i, \mathbf{p}_f \) are the initial and finite electron pulses, \( \mathbf{k} \) is the wave vector of a photon.

3. Structure factor
The structure factor of a medium in a three-dimensional case (a three-dimensional monocrystal, the angle brackets mean averaging over atom positions):
\[
\left\{ \sum_{j,i} \exp (i \mathbf{q} (\mathbf{r}_j - \mathbf{r}_i)) \right\} = N \left( 1 - \exp (-u^2 q^2) \right) + N_{\text{cell}} (2\pi)^3 \sum_{\mathbf{g}} e^{-i\mathbf{q}\cdot\mathbf{r}} |S(\mathbf{g})|^2 \delta^{(3)} (\mathbf{q} - \mathbf{g}),
\]

(2)

where \( N = N_0 N_{\text{cell}} \) is the full number of atoms in the volume of interaction, \( N_0 \) is the full number of cells in the volume of interaction, \( N_{\text{cell}} \) is the number of atoms in a cell, \( \mathbf{g} \) is the wave vector of a reciprocal lattice, \( S(\mathbf{q}) \) is the normalized structure factor of a unit cell of a crystal on the wave vector \( \mathbf{q} \), \( S(q = 0) = 1 \) (M.L. Ter-Mikhaelyan [4] uses a nonnormalized structure factor of a cell), \( n_a = N_{\text{cell}} / \Delta_{\text{cell}} \) is the volume concentration of atoms, \( \Delta_{\text{cell}} \) is the volume of a unit cell,

\( \delta^{(3)} (\mathbf{q}) = \delta (q_x) \delta (q_y) \delta (q_z) \) is the three-dimensional delta function of the wave vector transferred to the target.

In going to a two-dimensional case (we assume that a two-dimensional single crystal lies in the \( xy \) plane, the \( z \) coordinate is fixed: \( z = z_0 \); graphene), when \( \mathbf{q} \mathbf{r}_j = q_z z_0 + q_\| \mathbf{c}_j \), by analogy with the three-dimensional case for the structure factor of the target we have

\[
\left\{ \sum_{i,j} \exp (i q_\| (\mathbf{c}_j - \mathbf{c}_i)) \right\} = N \left( 1 - \exp (-u^2 q^2) \right) + N_{\text{cell}} (2\pi)^2 \sum_{\mathbf{g}} e^{-i\mathbf{q}\cdot\mathbf{r}} |S(\mathbf{g})|^2 \delta^{(2)} (q_\| - \mathbf{g}),
\]

(3)

where \( \mathbf{c}_j \) is the radius vector of an atom in the plane of the two-dimensional crystal, \( \mathbf{c} = (x, y) \), \( \delta^{(2)} (q_\|) = \delta (q_x) \delta (q_y) \) is the two-dimensional delta function, \( n_\| \) is the two-dimensional concentration of atoms, \( u \) is the root-mean-square deviation of atoms from the equilibrium position.

For a three-dimensional case we have

\[
\left\langle u^2 \right\rangle = \frac{3\hbar^2}{4M_a T_D} \left[ 1 + 4 \left( \frac{T}{T_D} \right)^2 \int_0^{T_D} \frac{y dy}{e^y - 1} \right],
\]

(4)

where \( T_D \) is the Debye temperature in energy units, \( M_a \) is the mass of atoms of a substance. For a three-dimensional lattice such as diamond \( u (C, T = 293^\circ K) = 0.041 \ \text{Å} \ (T_D = 1860^\circ K) \).

\( a = \sqrt{3} a_0 = 0.246 \ \text{nm} \) is the lattice constant for graphene, \( a_0 = 0.142 \ \text{nm} \) is the distance between the nearest atoms.

Structure factor of unit cell of graphene is

\[
|S(\mathbf{g})|^2 = \frac{1}{2} \left[ 1 + \cos \left( \frac{2\pi}{3} (2n_1 + n_2) \right) \right],
\]

where the modulus of the graphene reciprocal lattice vector – \( g(n_1, n_2) = \frac{4\pi}{\sqrt{3} a} \sqrt{n_1^2 + n_2^2 + n_1 n_2} \), \( n_{1,2} \) are the integers.

4. Polarization Bremsstrahlung on graphene

Let us consider polarization bremsstrahlung (PB) [1] arising as a result of electron scattering by the two-dimensional plane of graphene. The process geometry is shown in figure 1, where \( \alpha \) is the angle of photon emission with respect to the normal to the plane of graphene, \( \psi \) is the polar angle of electron incoming with respect to the normal to the plane of graphene), \( \varphi \) is the azimuth angle of electron incoming.
The cross-section of PB on an atom is
\[
\frac{d\sigma_{a}^{(PB)}}{d\omega d\Omega_{k}} = \frac{e^2}{\hbar} \frac{c}{\nu v} \int \delta(\omega - k \cdot v + q \cdot v) \left[ \frac{s \cdot \omega v / c^2 - q}{(q^2 - 2k \cdot q)} \right] \left( \frac{\omega}{c} \right)^2 \alpha(\omega, q) d\Omega_{q},
\]
where \( \alpha(\omega, q) \) is the generalized dynamic polarizability of an atom, \( s = k / |k| \) is the unit vector in the direction of photon emission. In the multiplicative approximation the generalized dynamic polarizability of an atom is expressed in terms of dipole polarizability and an atomic form factor: \( \alpha(\omega, q) = \alpha(\omega) \cdot F(q) \), where \( F(q) \) is the atomic form factor normalized by the condition \( F(q = 0) = 1 \).

4.1. Incoherent PB on graphene
The cross-section of incoherent PB on a target (in terms of one atom) is
\[
\frac{1}{N} \frac{d\sigma_{incoh}^{(PB)}}{d\omega d\Omega_{k}} = \frac{2 e^2}{\pi \nu v^2 c^3 \hbar \nu} \int_{q_{min}}^{q_{max}} dq I_p(q, v, \omega, \theta) \left( 1 - e^{-q^2} \right) \left( \frac{\omega^2}{c^2} \alpha(\omega, q) \right)^2,
\]
where \( q_{min}(\omega, v, \theta) = \frac{\omega}{\nu} \left( 1 - \frac{v}{c} \cos \theta \right) \), \( q_{max} = 2 \mu v \), \( \mu \) is the reduced mass of an electron and an atom of the target, \( \theta = \text{angle}(k, v) \) is the angle of emission.

\[
I_p(q, v, \omega, \theta) = \frac{q^3 \nu}{2 \pi} \int d\Omega_{q} \delta(\omega - k \cdot v + q \cdot v) \left[ \frac{s \cdot \omega v / c^2 - q}{(q^2 - 2k \cdot q)} \right]^2
\]

is the dimensionless kinematic integral, \( d\Omega_{q} \) is the element of the solid angle around the vector \( q \).

4.2. Coherent PB on graphene
The cross-section of coherent PB on a two-dimensional target (in terms of one atom) is
In derivation of this expression it was taken into account that integration over the two-dimensional delta function \( \delta^{(2)}(\mathbf{q}_\parallel - \mathbf{g}) \) gives \( \mathbf{q}_\parallel = \mathbf{g} \), and there remains integration over the component of the wave vector \( dq_z \) transferred to the target, this component being normal to the graphene plane, said integration is also “removed” at the expense of the presence of the delta function \( \delta(\omega - \mathbf{k} \cdot \mathbf{v} + \mathbf{g} \cdot \mathbf{v} + q_z v_z) \) under the integration sign. As a result, we find a fixed value for the normal (to the graphene plane) component of the wave vector transferred to the target as a function of the problem parameters:

\[
q_z = -g \tan \psi + \omega \frac{1 - (v/c) \cos \theta}{v \cos \psi}.
\]

This value should be substituted in the expression for the cross-section of coherent PB \( (|\mathbf{q}_\parallel| = q_z) \).

Taking into account that \( (\mathbf{q}_\parallel, \mathbf{g}) = 0 \), we obtain

\[
\frac{1}{N} \frac{d\sigma^{(PB)}_{coh}}{d\omega d\Omega_{\mathbf{k}}} = \frac{4\pi n_1}{\cos \psi} \left(\frac{e^2}{\hbar \omega}\right)^\frac{1}{2} \alpha(\omega) \frac{1}{\sqrt{c^2 v^2}} \sum_{\mathbf{g}} e^{-\omega^2 [g^2 + q_z^2]} \left| S(\mathbf{g}) \right|^2 \left| F\left(\sqrt{g^2 + q_z^2}\right) \right|^2 P(\mathbf{g}, \mathbf{k}, q_z),
\]

where

\[
P(\mathbf{g}, \mathbf{k}, q_z) = \left(\frac{\omega v}{c^2}\right)^2 + g^2 + q_z^2 - 2 \frac{\omega v}{c^2} (g \sin \psi + q_z \cos \psi) - \left[ \frac{\omega v}{c^2} \cos \theta - g \sin \alpha - q_z \cos \alpha \right]^2,
\]

\[
\left| S(\mathbf{g}) \right|^2 = \cos^2 \left(\frac{\pi}{3}(2n_1 + n_2)\right), |g| = g(n_1, n_2) = \frac{4\pi}{\sqrt{3} a} \sqrt{n_1^2 + n_2^2 + n_1 n_2},
\]

\[
\cos \theta = \cos \alpha \cos \psi + \cos \varphi \sin \alpha \sin \psi, n_z = \frac{4}{\sqrt{3} a^2}.
\]

Summation over the reciprocal lattice vectors \( \mathbf{g} \) implies summation over the integers \( n_{1,2} \) determining the modulus of the vector \( \mathbf{g} \). Let us note that in contrast to coherent PB in a three-dimensional monocrystal, when the emitted frequency is fixed by the condition \( \omega^{(3)}_{\max} = -\frac{g v}{1 - \beta \cos \theta} \),

here from we find for a cubic crystal: \( \omega^{(3)}_{\max} = -\frac{g v (n_1 \sin \psi \cos \varphi + n_2 \sin \psi \sin \varphi + n_z \cos \psi)}{1 - \beta \cos \theta} \), the frequency of coherent PB in a two-dimensional monocrystal is not a fixed value. Nevertheless, in a two-dimensional case with fulfillment of certain conditions (see below) the PB spectrum has sharp maxima.

For the denominator of equation (11) taking into account the explicit form of \( q_z \), we find

\[
\frac{1}{\sqrt{c^2 v^2}} \sum_{\mathbf{g}} e^{-\omega^2 [g^2 + q_z^2]} \left| S(\mathbf{g}) \right|^2 \left| F\left(\sqrt{g^2 + q_z^2}\right) \right|^2 P(\mathbf{g}, \mathbf{k}, q_z).
\]
\[
\frac{g^4}{\cos^4 \psi} \left(\frac{\omega}{g v}\right)^2 \delta \left[\delta - 2 \beta \cos \alpha \cos \psi\right] + 2 \beta \frac{\omega}{g v} \cos \psi \left[\cos \alpha \sin \psi - \sin \alpha - \frac{\delta}{\beta} \tan \psi\right] + 1 \right)^2, \quad (14)
\]

where \( \delta = 1 - \beta \cos \theta \), \( \beta = v/c \). For the zero angle of electron incoming into the graphene plane (\( \psi = 0 \)) the expression for the denominator is simplified to look like

\[
\text{Den} \left( \omega, \alpha, \psi = 0, \beta, \theta = \alpha \right) = g^4 \left(\frac{\omega}{g v}\right)^2 \left(1 - \beta \cos \alpha\right) \left(1 - 3 \beta \cos \alpha\right) - 2 \beta \frac{\omega}{g v} \sin \alpha + 1 \right)^2. \quad (15)
\]

The resonance condition in the cross-section of coherent PB in the general case is \( \text{Den} \left( \omega, \alpha, \psi, \beta, \theta \right) = 0 \). If this equation is solved with respect to the emission frequency, the following expression for the frequency of a spectral maximum in coherent PB on graphene will be obtained: \( \omega_{\text{max}} = g v F_\omega (\alpha, \psi, \theta, \beta) \). Here the dimensionless function is introduced:

\[
F_\omega (\alpha, \psi, \theta, \beta) = \frac{\cos \psi \left(\beta \sin \alpha + \frac{\delta}{\beta} \tan \psi - \beta \sin \psi \cos \alpha\right) + \text{sign} \left(\delta - 2 \beta \cos \alpha \cos \psi\right) \sqrt{D}}{\delta \left(\delta - 2 \beta \cos \alpha \cos \psi\right)}, \quad (16)
\]

\[
D = \cos^2 \psi \left(\beta \sin \alpha + \frac{\delta}{\beta} \tan \psi - \beta \sin \psi \cos \alpha\right)^2 - \delta \left(\delta - 2 \beta \cos \alpha \cos \psi\right). \quad (17)
\]

In case of the zero angle of electron incoming (\( \psi = 0 \)) into a two-dimensional monocrystal, we have for the function determining the dependence of the resonance frequency of emission on the electron velocity and the angle of photon emission:

\[
F_\omega (\psi = 0) = \frac{\beta \sin \alpha + \text{sign} \left(1 - 3 \beta \cos \alpha\right) \sqrt{\left(\beta \sin \alpha\right)^2 - \left(1 - \beta \cos \alpha\right) \left(1 - 3 \beta \cos \alpha\right)}}{\left(1 - \beta \cos \alpha\right) \left(1 - 3 \beta \cos \alpha\right)}. \quad (18)
\]

Figure 2. The dependence of the determinant in the expression determining the resonance frequency of PB for the zero angle of electron incoming on the electron velocity for different angles of emission: solid line – \( \alpha = 0 \), dotted line – \( \alpha = \pi/4 \), dashed line – \( \alpha = \pi/3 \), dotted-dashed line – \( \alpha = \pi/2 \).
The total cross-section of electron PB on graphene in terms of one atom is equal to the sum of the incoherent and coherent parts. The comparison of the cross-sections (in terms of one atom) of coherent and incoherent PB on graphene and on a carbon atom for the normal incidence of an electron on the graphene plane ($\psi=0$), and an angle of emission of $30^\circ$ are given in figures 3 and 4.

![Figure 3](image-url)

**Figure 3.** For an electron energy of 30 keV ($\nu = 45$ atomic units): solid line – coherent PB, dotted line – incoherent PB, dashed line – atomic PB.

![Figure 4](image-url)

**Figure 4.** For an electron energy of 4 MeV ($\nu = 136$ atomic units): solid line – coherent PB, dotted line – incoherent PB, dashed line – atomic PB.

The dependence of the cross-section of coherent PB on graphene on the angle of electron incoming, for an electron energy of 58 keV (velocity $\nu = 60$ atomic units), $\alpha = 30^\circ$ and different photon energies is shown in figure 5.
5. Static (ordinary) Bremsstrahlung on graphene

For calculation of the coherent part of SB on graphene it is necessary to express the cross-section of the process on an atom [6] in terms of an integral over the transferred wave vector $q$. Then the expression for the differential cross-section of coherent SB on graphene (in terms of one atom) looks like

$$
\frac{1}{N} \frac{d\sigma^{coh}_{OB}}{d\omega d\Omega_k} = \frac{2n_z}{\cos\psi} \frac{Z^2 e^6 (1+\cos^2\theta) \left(1 - \frac{v}{c}\right)^2}{\hbar \omega m^2 v^2 c^3 \left(1 - \frac{v}{c} \cos\theta\right)^2} \sum_g e^{-i\omega (g^2 + q_z^2)} S(g)^2 \left|1 - F(\sqrt{g^2 + q_z^2})\right|^2,
$$

(19)

In view of the last equation summation over the reciprocal lattice vectors $g$ in this formula reduces to summation over the set of the integers $(n_1, n_2)$ - see formulas (12).

For the incoherent part of the cross-section of SB on graphene (in terms of one atom) we have

$$
\frac{1}{N} \frac{d\sigma^{incoh}_{OB}}{d\omega d\Omega_k} \approx \frac{1}{\pi} \frac{Z^2 e^6 (1+\cos^2\theta) \left(1 - \frac{v}{c}\right)^2}{m^2 \hbar \omega v^2 c^3 \left(1 - \frac{v}{c} \cos\theta\right)^2} \int_{q_{min}} q_{max} \left(1 - \exp\left(-u^2 q^2\right)\right) dq.
$$

(20)

6. Conclusion

Polarization Bremsstrahlung (PB) and Static (ordinary) Bremsstrahlung (SB) of fast electron scattered on graphene are investigated theoretically. The coherent and incoherent interactions between electron and two-dimensional graphene lattice so as dynamical polarizability and form-factor of carbon atom core are taken into account.

It is shown that spectral features of PB cross section are depended on electron velocity, projectile incident angle and radiation angle. In specified region of the problems parameters sharp maxima in PB
spectrum is predicted. For normal electron incidence on graphene plane the analytical description of resonance frequencies on velocity and radiation angles is obtained.

In low frequency range coherent PB is dominated by the process without momentum exchange between projectile and graphene. In this range coherent PB is comparable or greater than the incoherent one. Our analysis show that dominated Bremsstrahlung channels of fast electron on graphene are coherent PB and incoherent SB.

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