Bremsstrahlung of fast electron on graphene

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Fig.1. Static and Polarization Channels of Bremsstrahlung.
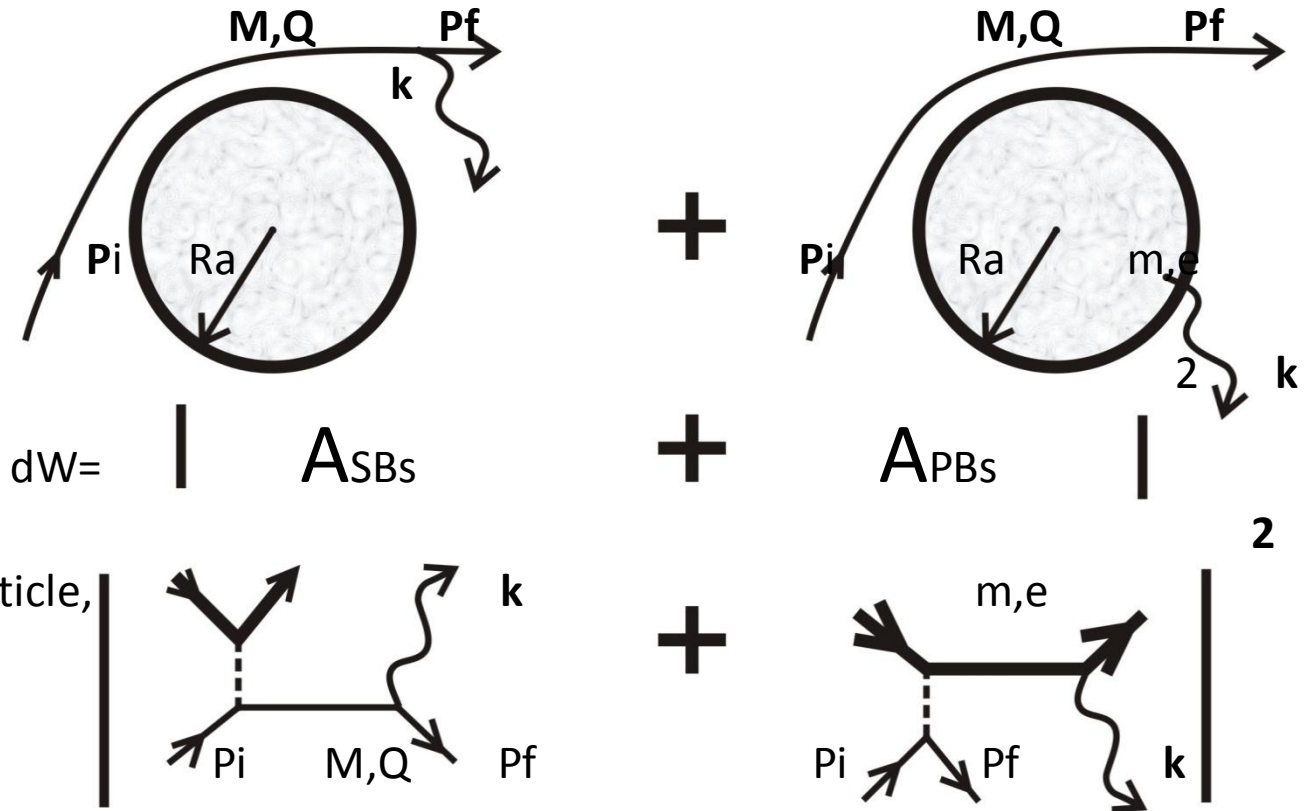
P,M,Q-momentum, mass and charge of a projectile;

k – momentum of

a Bs photon,

Ra – atomic radius,

⟶ -projectile particle,

⟹ -target particle.

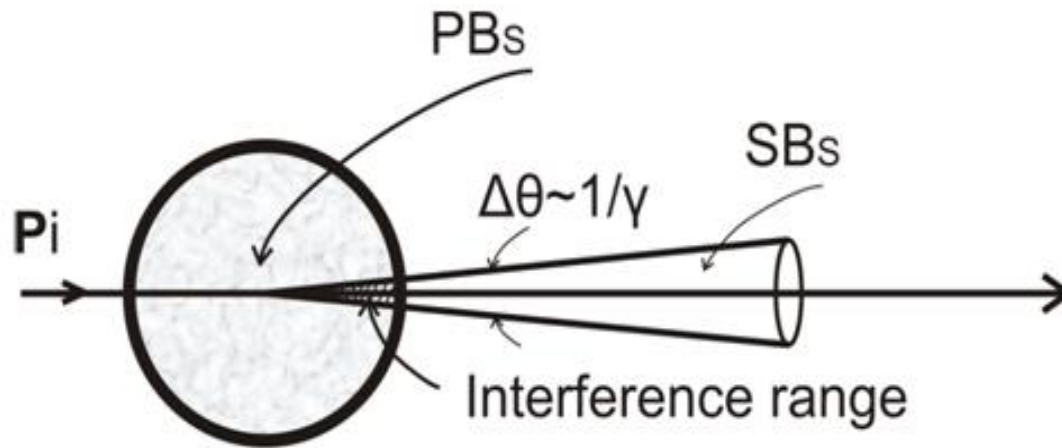$$dW = \left| A_{SBs} \right| + \left| A_{PBs} \right|^2$$

Fig.2. Directional diagram of PBs and SBs from ultrarelativistic ($\gamma \gg 1$) projectile on atom.

For relativistic projectile particles the essential distinction in the bremsstrahlung directional diagrams for both channels was shown on Fig. 2. A relativistic projectile emits in a narrow cone of angles $\Delta\theta \sim Mc^2/E \sim 1/\gamma$ along its momentum, while the polarization of target electrons emits practically isotropically, and this allows the interference contribution of both bremsstrahlung channels in the ultra-relativistic case to be neglected

3-D crystal

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

$$d\sigma_{t\arg et} = \left| \sum_j \exp\left(i\mathbf{q}\,\mathbf{r}_j\right) \right|^2 d\sigma_{atom} \qquad (1),$$

where the sum is over all target atoms being in the volume of interaction, $d\sigma_{atom}$ is the differential cross-section of the process on one atom. The structure factor of a medium in a three-dimensional case (a three-dimensional single crystal, the angle brackets mean averaging over atom positions):

$$\left\langle \sum_{j,j'} \exp\left(i\mathbf{q}\left(\mathbf{r}_j - \mathbf{r}_{j'}\right)\right) \right\rangle = N\left(1 - \exp\left(-u^2\,q^2\right)\right) + N\,n_a\left(2\pi\right)^3 \sum_{\mathbf{g}} e^{-u^2 g^2} \left|S\left(\mathbf{g}\right)\right|^2 \delta^{(3)}\left(\mathbf{q} - \mathbf{g}\right) \quad (2),$$

where N is the full number of atoms in the volume of interaction, $\mathbf{g}$ 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($\mathbf{q}$=0)=1, u^2 is the mean square of thermal displacement of an atom.
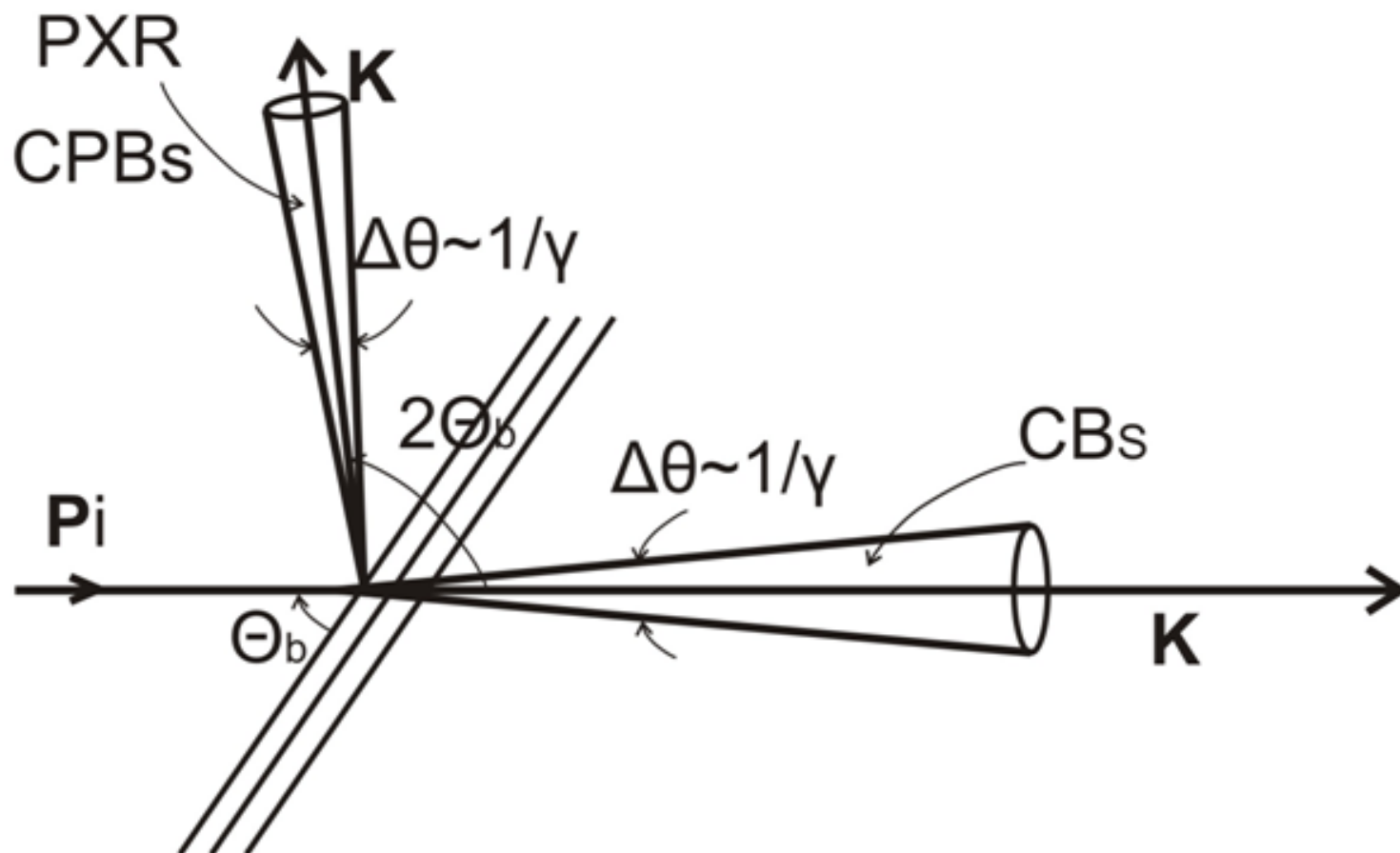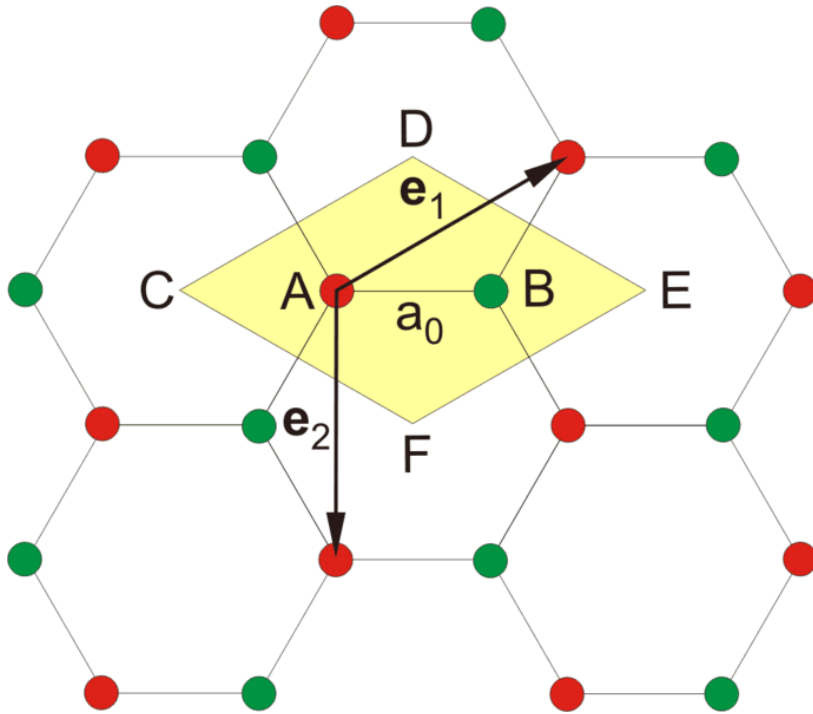
Fig.3. Directional diagrams of PXR=CPBs and CBs=CSBs from ultrarelativistic (γ >>1) projectile in crystal.

2D crystal – graphene

Fig. 4. The crystal structure of graphene.

A unit cell (CDEF) and elementary translation vectors ($\mathbf{e}_1$, $\mathbf{e}_2$) are shown

$a = \sqrt{3}\, a_0 = 0.246$ nm is the lattice constant for graphene, $a_0 = 0.142$ nm is the distance between the nearest atoms (the distance between the atoms in a unit cell, graphene has *two atoms* in a unit cell).

Structure factor of unit cell of graphene

- We assume that an atom A is at the origin

- of the coordinates, then

$$S(\mathbf{q}) = \frac{1}{2}\left[1 + \exp\left(i\,\mathbf{q}\,\mathbf{r}_B\right)\right]$$

- It follows from the figure that

$$\mathbf{r}_B = \frac{2}{3}\mathbf{e}_1 + \frac{1}{3}\mathbf{e}_2$$

- Then for the vectors of the reciprocal lattice of graphene we have

$$\mathbf{g}_1 = \left(4\pi/\sqrt{3}\,a, 0\right) \quad , \quad \mathbf{g}_2 = \left(2\pi/\sqrt{3}\,a, 2\pi/a\right)$$

and the structure factor of a unit cell of graphene is

$$S(\mathbf{g}) = \frac{1}{2}\left[1 + \exp\left(i\left(2n_1 + n_2\right)\frac{2\pi}{3}\right)\right]$$

Here from we find

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

Generalized dynamic polarizability of a carbon atom

- The sum over the virtual states of atomic electrons can be expressed in terms of the generalized dynamic atom polarizability $\alpha(\mathbf{q}, \omega)$ that shows a resonance nature at atomic frequencies.

- In the multiplicative approximation the generalized dynamic polarizability of an atom is expressed in terms of dipole polarizability and an atomic form factor:

$$\alpha(\omega, \mathbf{q}) = \alpha(\omega)\tilde{F}(q) \qquad (4),$$

- the atomic form factor is calculated on the Slater wave functions of atomic orbitals for carbon.

- $\tilde{F}(q) = \dfrac{1}{Z}\sum_j N_j\, Q(q, \beta_j, \mu_j)$, $Q(q, \beta, \mu) = \dfrac{\left[1 + (q/2\beta)^2\right]^{\mu}}{(\mu\ q/\beta)}\sin\left[2\ \mu\ arctg\left(\dfrac{q}{2\ \beta}\right)\right]$ (5)

To obtain the frequency dependence of the imaginary part of the dipole polarizability, we proceed from its relation with the emission absorption cross-section given by the optical theorem:

$$\text{Im}\big(\alpha(\omega)\big) = \frac{c}{4 \ \pi \ \omega} \ \sigma_{ph}(\omega)$$

The data on the emission absorption coefficient given at the site of the Berkeley National Laboratory are used.
The real part of the atom polarizability can be restored with the use of the Kramers-Kronig relation.

Bremsstrahlung of electron scattering by the two-dimensional plane of graphene.
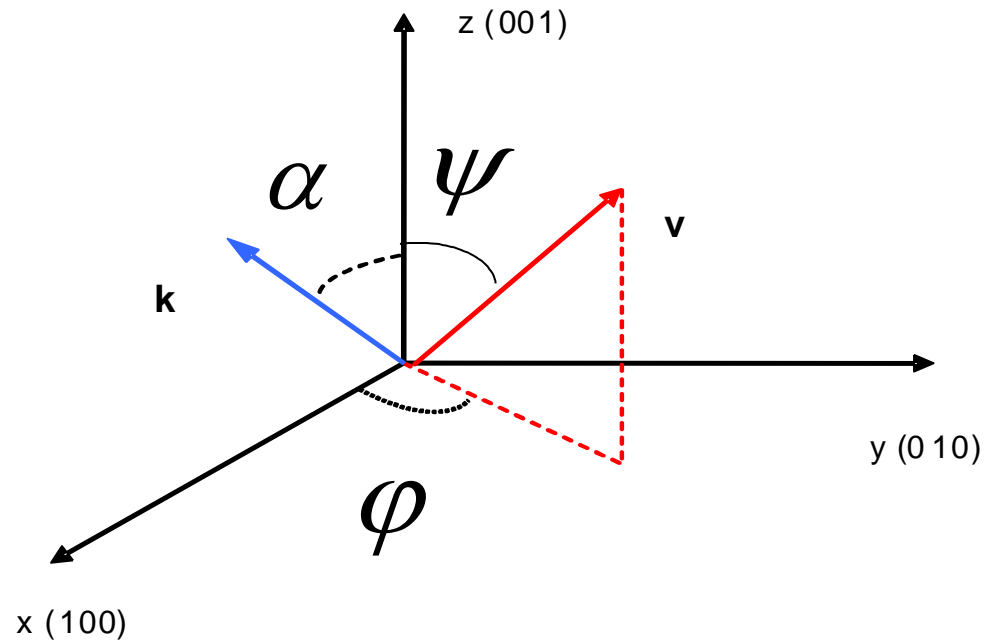
The process geometry is shown in Fig. 5

α is the angle of photon emission with respect to the normal to the plane of graphene,

ψ is the polar angle of electron incoming with respect to the normal to the plane of graphene,

φ is the azimuth angle of electron incoming.

Incoherent PB on graphene

The cross-section of incoherent PB on a target (in terms of one atom) is

- $\dfrac{1}{N}\dfrac{d\sigma^{(PB)}_{incoh}}{d\omega\,d\Omega_{\mathbf{k}}} = \dfrac{2e^2}{\pi\,\mathrm{v}^2\,\mathrm{c}^3\,\hbar\omega}\int\limits_{q_{\min}}^{q_{\max}}\dfrac{dq}{q}\,I_\varphi\left(q,\mathrm{v},\omega,\theta\right)\left(1-e^{-u^2 q^2}\right)\left|\omega^2\,\alpha\left(\omega,q\right)\right|^2$ (6)

- where $q_{\min}\left(\omega,\mathrm{v},\theta\right)=\dfrac{\omega}{\mathrm{v}}\left(1-\dfrac{\mathrm{v}}{c}\,\cos\theta\right)$, $q_{\max}=2\mu\,\mathrm{v}$,

- μ is the reduced mass of an electron and an atom of the target,

- $\theta = angle\left(\mathbf{k},\mathbf{v}\right)$

- $I_\varphi\left(q,\mathrm{v},\omega,\theta\right)=\dfrac{q^3\,\mathrm{v}}{2\pi}\int d\Omega_{\mathbf{q}}\,\delta\left(\omega-\mathbf{kv}+\mathbf{qv}\right)\dfrac{\left[\mathbf{s},\omega\mathbf{v}/c^2-\mathbf{q}\right]^2}{\left(\mathbf{q}^2-2\,\mathbf{k}\,\mathbf{q}\right)^2}$ (7)

Coherent PB on graphene

- The cross-section of coherent PB on a two-dimensional target (in terms of one atom) is

- $$\frac{1}{N}\frac{d\sigma_{coh}^{(PB)}}{d\omega\,d\Omega_{\mathbf{k}}} = \frac{4\pi n_s}{\cos\psi}\left(\frac{e^2}{\hbar\omega}\right)\frac{\omega^4\left|\alpha(\omega)\right|^2}{c^3\,\mathrm{v}^2}\sum_{\mathbf{g}} e^{-u^2\left(g^2+q_z^2\right)}\left|S(\mathbf{g})\right|^2\left|\tilde{F}\left(\sqrt{g^2+q_z^2}\right)\right|^2 P(\mathbf{g},\mathbf{k},\mathbf{q}_\perp)$$

$$(8)$$

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

- $$(9)$$

- $$\cos\theta = \cos\alpha\cos\psi + \cos\varphi\sin\alpha\sin\psi \ , \quad n_s = \frac{4}{\sqrt{3}\,a^2}$$

- $$q_z = -g\,tg\psi + \omega\frac{1-(\mathrm{v}/c)\cos\theta}{\mathrm{v}\cos\psi}$$

$$(10)$$

Frequency of a spectral maximum in coherent PB on graphene

- The resonance condition in the cross-section of coherent PB in the general case gives:

- $$\omega_{\max} = g\, \text{v}\, F_{\omega}\left(\alpha, \psi, \theta, \beta\right) \qquad (11)$$

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

$$F_{\omega}\left(\psi = 0\right) = \frac{\beta \sin\alpha + \text{sign}\left(1 - 3\beta\cos\alpha\right)\sqrt{\left(\beta\sin\alpha\right)^{2} - \left(1 - \beta\cos\alpha\right)\left(1 - 3\beta\cos\alpha\right)}}{\left(1 - \beta\cos\alpha\right)\left(1 - 3\beta\cos\alpha\right)} \qquad (12)$$

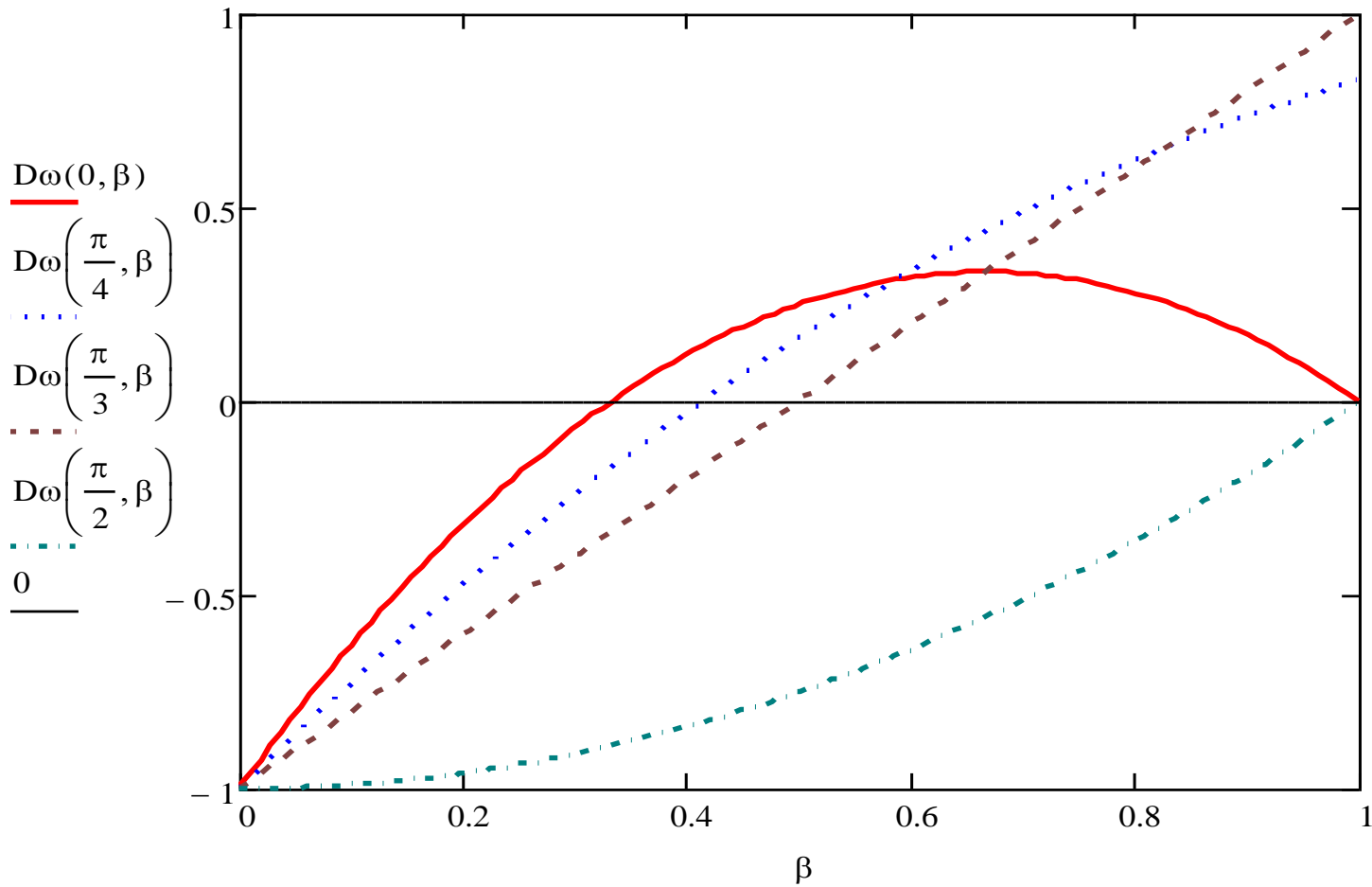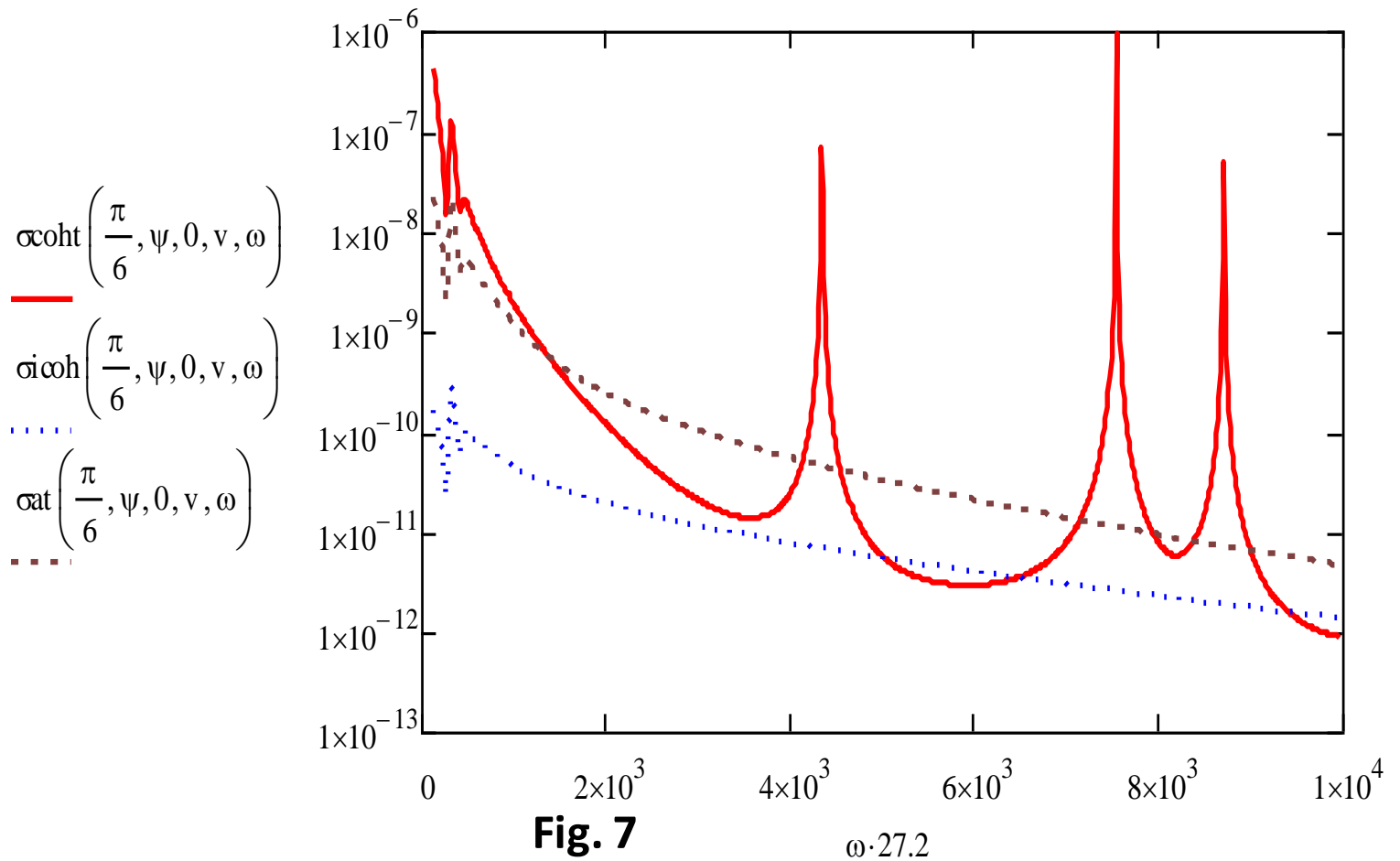**Fig. 6**

The dependence of the determinant in the expression (12) on the electron velocity (β) for different angles of emission (α).

Fig. 7

$$\sigma_{coht}\left(\frac{\pi}{6}, \psi, 0, v, \omega\right)$$

$$\sigma_{icoh}\left(\frac{\pi}{6}, \psi, 0, v, \omega\right)$$

$$\sigma_{at}\left(\frac{\pi}{6}, \psi, 0, v, \omega\right)$$

$\omega \cdot 27.2$

The comparison of the cross-sections of coherent and incoherent PB on graphene and on a carbon atom for an electron energy of 58 keV (v = 60 atomic units, the normal incidence of an electron on the graphene plane (ψ=0), and an angle of emission of 30°).
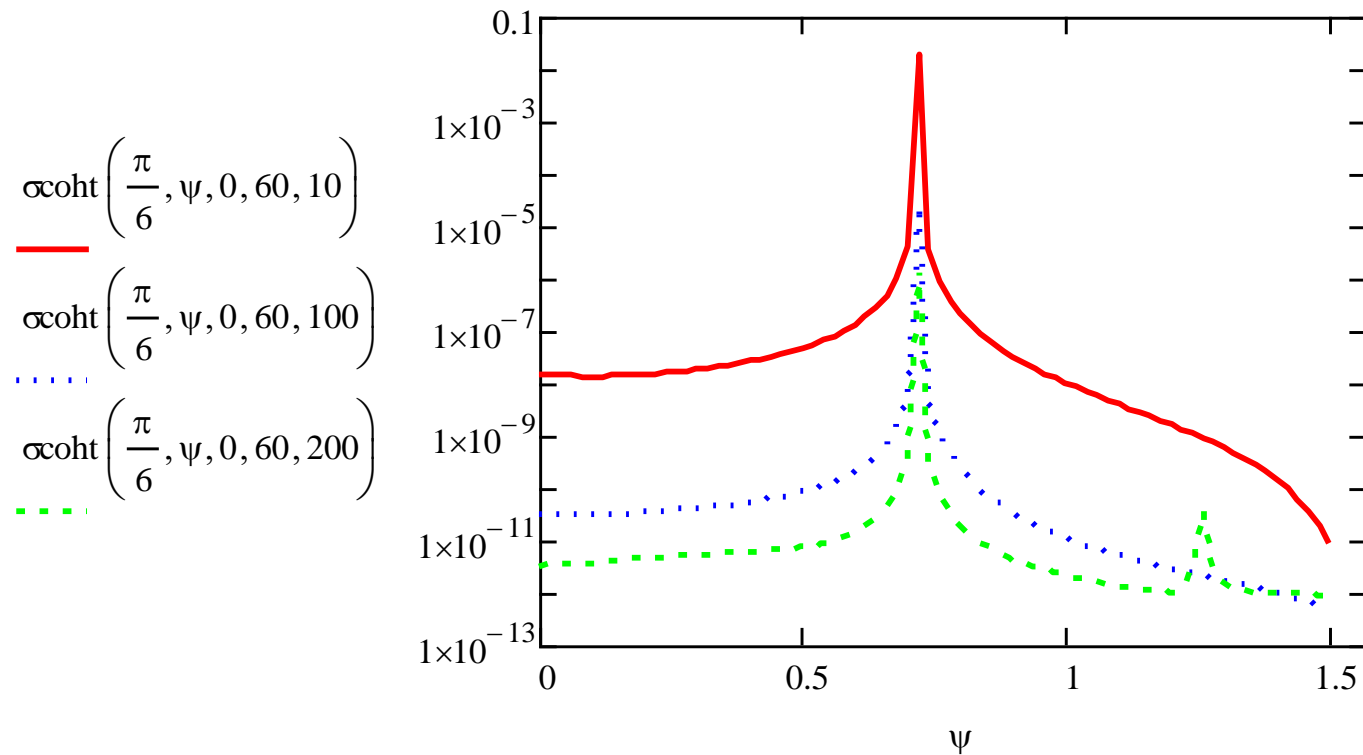
Fig. 9.

The dependence of the cross-section of coherent PB on graphene on the angle of electron incoming, $\alpha=30°$, for the electron velocity v = 60 atomic units (energy = 58 keV) and different photon energies.

Coherent static (ordinary) bremsstrahlung on graphene

The expression for the differential cross-section of coherent SB on graphene is:

$$\frac{1}{N}\frac{d\sigma_{coh}^{(OB)}}{d\omega\, d\Omega_{\mathbf{k}}} = \frac{2n_s}{\cos\psi}\frac{Z^2 e^6\left(1+\cos^2\theta\right)\left(1-\left(\frac{v}{c}\right)^2\right)}{\hbar\,\omega\, m^2\, v^2\, c^3\left(1-\frac{v}{c}\cos\theta\right)^2}\sum_{\mathbf{g}} e^{-u^2\left(g^2+q_z^2\right)}\left|S(\mathbf{g})\right|^2\frac{\left[1-\tilde{F}\left(\sqrt{g^2+q_z^2}\right)\right]^2}{g^2+q_z^2} \qquad (13)$$

where
$$q_z = -g\, tg\psi + \omega\frac{1-\left(v/c\right)\cos\theta}{v\cos\psi}\,,$$

$$\left|\mathbf{g}\right| = g\left(n_1, n_2\right) = \frac{4\pi}{\sqrt{3}\,a}\sqrt{n_1^2+n_2^2+n_1\, n_2}$$
.

Summation over the reciprocal lattice vectors **g** in the formula (13) reduces to summation over the set of the integers (n_1, n_2) .

Incoherent static (ordinary) bremsstrahlung on graphene

- **For the incoherent part of the cross-section of SB on graphene we have**

$$\frac{1}{N}\frac{d\sigma^{OB}_{incoh}}{d\omega\, d\Omega_{\mathbf{k}}} \approx \frac{1}{\pi} \frac{Z^2 e^6 \left(1+\cos^2\theta\right)\left(1-\left(\frac{\mathrm{v}}{c}\right)^2\right)}{m^2\,\hbar\,\omega\,\mathrm{v}^2\, c^3 \left(1-\frac{\mathrm{v}}{c}\cos\theta\right)^2} \int\limits_{q_{min}}^{q_{max}} \frac{\left(1-\tilde{F}(q)\right)^2}{q}\left(1-\exp\left(-u^2\, q^2\right)\right)dq \quad (14)$$

The difference of incoherent channels of PB and SB on graphene (Fig. 15) is about two and a half orders of magnitude at the maximum of the spectral dependence of PB. The latter fact is connected with the fact that the polarization channel is formed at great distances from a target, the contribution of these distances to incoherent emission is suppressed by the Debye-Waller factor that is small for q<1/u (high impact parameters).
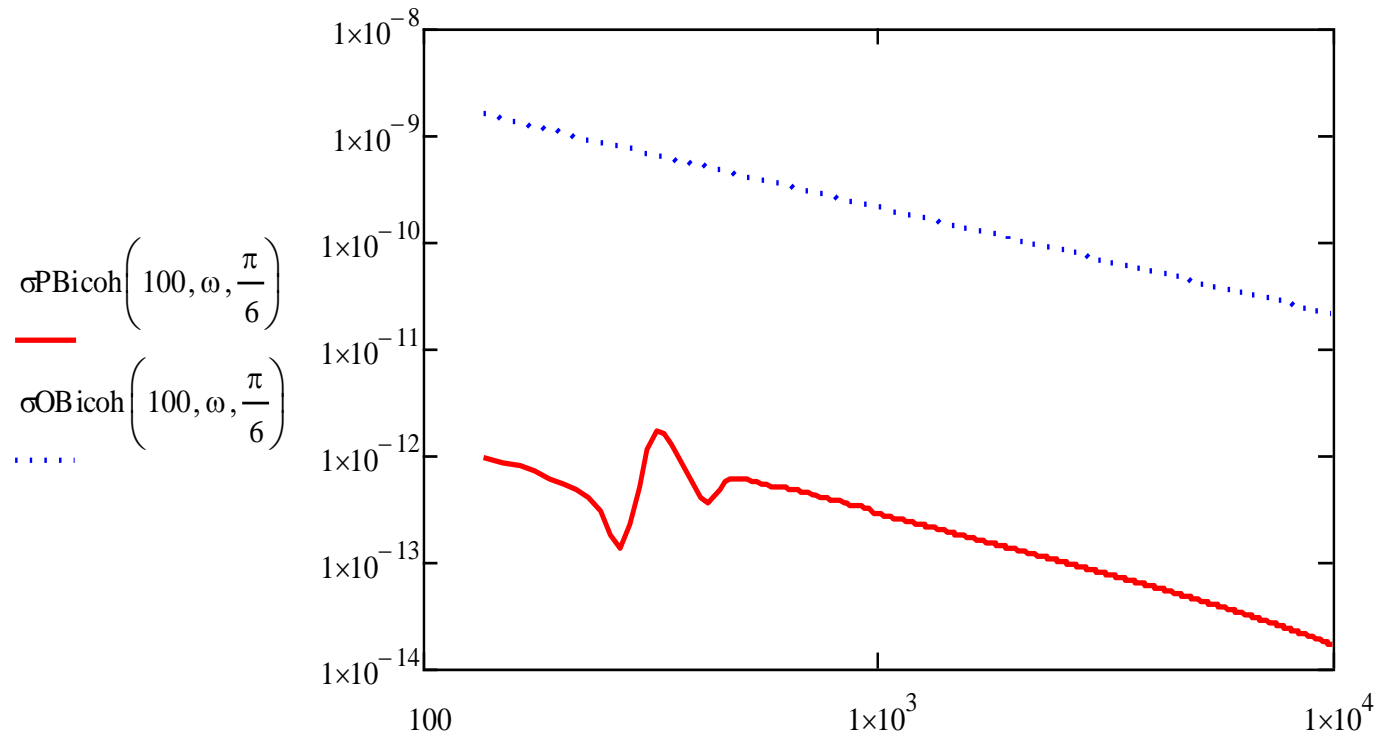
Fig. 10.

The comparison of the spectral cross-sections of incoherent PB (continuous red curve) and SB (dotted blue curve) of an electron scattered on graphene, v = 100 atomic units, (energy= 240 кэВ) the angle of emission is α=30°.

Results

- 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.

- 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.

- Our analysis show that dominated Bremsstrahlung channels of fast electron on graphene are coherent PB and incoherent SB.
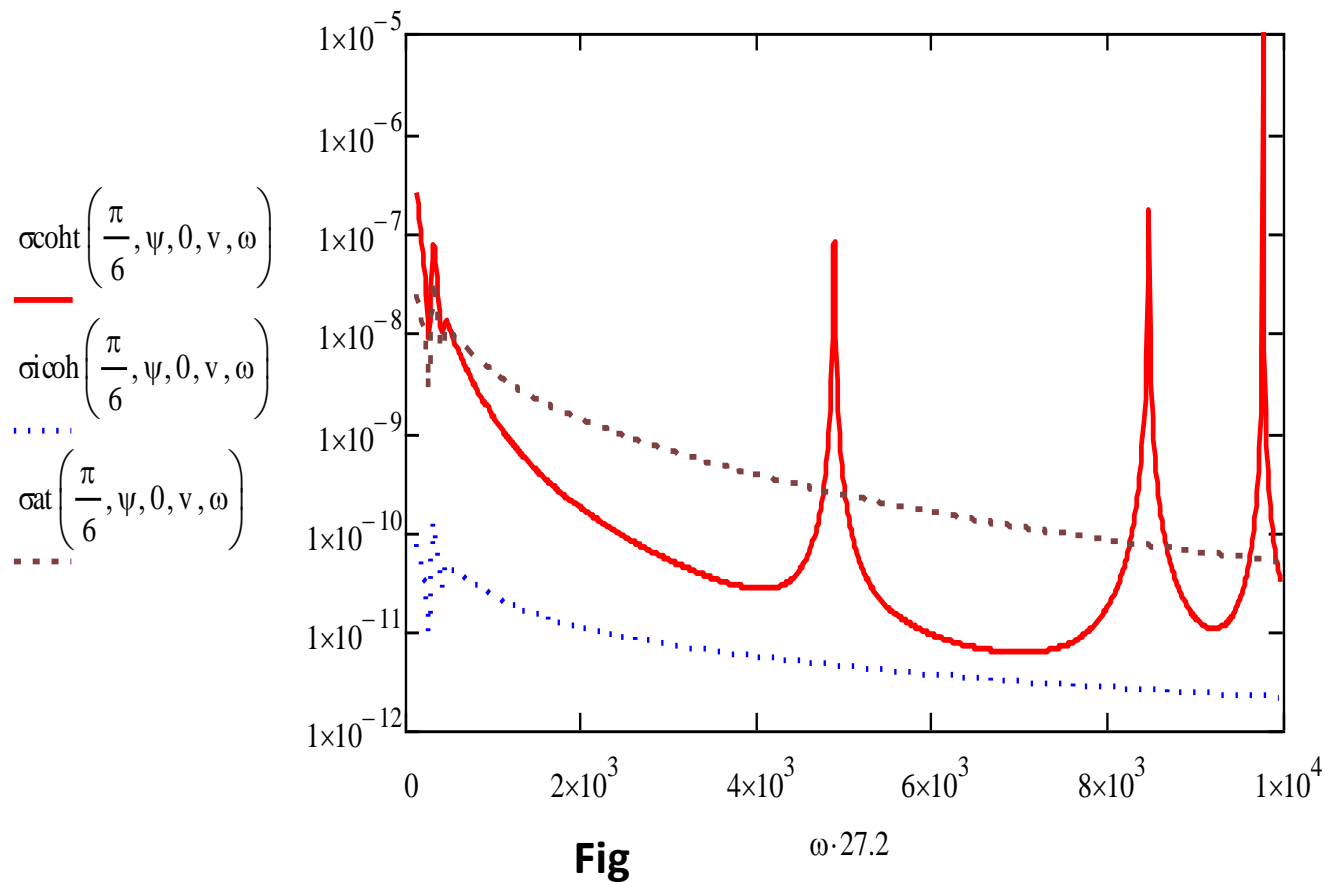
Fig

The comparison of the cross-sections of coherent and incoherent PB on graphene and on a carbon atom for an electron energy of 4 MeV (v = 136 atomic units), the normal incidence of an electron on the graphene plane (ψ=0), and an angle of emission of 30°.