Polarization bremsstrahlung from non-relativistic electrons penetrating a polycrystalline target

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Abstract

The bremsstrahlung theory in polycrystalline medium is developed on the basis of a quantum approach derived earlier for a separate atom. Polarization channel of bremsstrahlung have been taken into account. The doubly differential cross section with respect to radiation frequency and the angle of radiation is calculated without fitting parameters for the bremsstrahlung in polycrystalline silver. It is predicted that the periodic structure of the target and oscillations of the lattice atoms influence substantially on the radiation spectrum in the range of 1–5 keV for the electron with the energy of 50 keV.

Bremsstrahlung (BrS) theory created in the pioneering works of Sommerfeld, Bethe and Heitler (BH theory) and Sauter [1] and further developed in [2,3] assumes that radiating electron scatters in the static field of an atom or separated atomic nucleus. Later the limited character of such approach was established. Naturally, this approach does not account for the fact that not only incident electron but the atomic electrons also emit photon in the collision. In other words, it does not take account for the dynamic polarization of the atom appearing during the scattering process. Thus, the total BrS amplitude A^{at}_{fi} equals to the sum of static A^{st}_{fi} and polarization A^{pol}_{fi} terms:

$$A^{\mathrm{at}}_{fi} = A^{\mathrm{st}}_{fi} + A^{\mathrm{pol}}_{fi}. \tag{1}$$

Here the index "i" corresponds to the initial electron state with the energy E_i and momentum $\mathbf{p}_i$, the index "f" corresponds to the final electron state. Incident electron emits the photon with the energy ω and momentum $\mathbf{k}$. We use the system of units $\hbar = c = 1$.

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The importance of such approach in the BrS theory was demonstrated for the scattering of charged particle by atoms [4,5,7,9], plasmas [4,6] and solids [8,10]. The necessity of this approach follows, e.g., from the fact that in the case of electron scattering by many-electron atom one cannot obtain the correct transition to the case of classical physics and has not the correct physical picture of the phenomenon without the second term in the right-hand side of equality (1). The correct physical picture is next: radiation due the scattering of the incident electron on atomic electrons disappears in the high frequency limit within the framework of the first Born and dipole approximation with respect to the photon wavelength λ. This elimination is a consequence of the equal charge/mass (e/m) ratio for all—incident and atomic—electrons. Therefore, only the radiation due to the scattering of the incident electron by "stripped" nucleus remains. This effect at first predicted in [11] was named later as the effect of "descreening" [5, p. 72]. It was substantially generalized in [12, 4 Chapter 7] to the general case when the atom "stripping" occurs in a sequential manner—shell-by-shell—until only "stripped" nucleus remains.

The necessity to take into account the dynamic polarization of the atom in BrS theory is brightly demonstrated in the case of a proton or other heavy particle (with mass M) scattering by an atom. Then the ratio of the second to the first term in the right-hand side of Eq. (1) is of the order of M/m because the static and polarization amplitudes are proportional to the corresponding accelerations and consequently inversely proportional to masses of emitting particles [13].

At first time the polarization BrS (PBrS) was discovered experimentally in the special case when the atomic photoionization spectrum has a broad maximum, so-called "giant" resonance. Corresponding resonance arises in PBrS spectrum due to virtual transitions of atomic electrons in the same region of continuum energy spectrum where the "giant" resonance takes place [5]. The relative measurements of BrS spectrum are sufficient for the detection of this resonance [14]. At the same time, PBrS may be observed in more general case when "giant" resonance is absent as it is in PBrS on hydrogen and many other atoms [15,16].

Recently Quarles and Portillo made the absolute measurements of the doubly differential BrS (with respect to the BrS frequency and solid angle of the emitted photon observation) of non-relativistic electrons scattered by noble gas atoms [17]. In these experiments the deviation from the BH theory was clearly observed. New level of the experiment makes the following question of the topical interest: is it possible to detect the deviation from BH theory for BrS of non-relativistic electron in crystalline solids? This question was studied already for BrS generated by relativistic electrons when photon is formed along the long part of the emitting electron trajectory—"coherence length" or "formation length"—in crystalline and amorphous targets [18–21]. Influence of the medium was taken into account for each of two terms in the right-hand side of Eq. (1) separately and simultaneously [18,22–25].

Since the radiation probability is proportional to the squared modulus of the expression (1) the interference between static and polarization BrS amplitudes should be taken into account. This is true for the BrS on atoms [11,15,26] and on solids [24,25].

Let us consider BrS of non-relativistic electron scattered by a single microcrystal of the polycrystalline target. Obviously, in this case the BrS amplitude is equal to the sum of the amplitudes on separate atoms. BrS amplitude for the atom situated in the given point of crystalline lattice can be obtained from the amplitude for separate atom with the use of the translation operator T_{ξ} which transfers atom from the given lattice point in another point connected with the first point by vector $\boldsymbol{\xi}$. Thus BrS amplitude for crystalline target is equal to:

$$A^{\text{cr}}_{fi} = \sum_{\xi} T_{\xi} A^{\text{at}}_{fi}(0),$$

$$T_{\xi} A^{\text{at}}_{fi}(0) = A^{\text{at}}_{fi}(0)\exp(i\mathbf{q}_1\mathbf{r}_j),$$

$$\mathbf{q}_1 = \mathbf{p}_i - \mathbf{p}_f - \mathbf{k}, \qquad (2)$$

where $A^{\text{at}}_{fi}(0)$ is the BrS amplitude for the atom situated in the origin of Cartesian coordinate system, axes of this coordinate system are assumed to coincide with the crystallographic axes of the cubic crystal, $\mathbf{r}_j$ is Cartesian coordinate of jth atom. Summation is drawn up over all possible atomic positions in the lattice elementary cell and over all elementary cells of the microcrystal. The amplitude of one-photon BrS for separate atom is calculated in the first Born approximation for electron–target scattering and in the first order of perturbation theory with respect to the interaction between incident and atomic electrons with radiation.

The expression of the BrS cross section is factorized and the factor describing the lattice influence on BrS after averaging over the thermal lattice oscillations takes the following form:

$$\overline{\left|\sum_j \exp(i\mathbf{q}_1\mathbf{r}_j)\right|^2} = N\left(1 - e^{-q_1^2\overline{u^2}}\right) + N_0\frac{(2\pi)^3}{\Delta}\sum_{\mathbf{g}} e^{-g^2\overline{u^2}}\left|S(\mathbf{g})\right|^2\delta(\mathbf{q}_1 - \mathbf{g}), \qquad (3)$$

here, N is the total number of the target atoms in the interaction volume, N_0 is the number of elementary cell in this volume, Δ is the volume of elementary cell, $S(\mathbf{g})$ is the structure factor of lattice elementary cell [27], $\mathbf{g}$ is the reciprocal lattice vector, ($g_i = \frac{2\pi}{a}n_i$, n_i is an integer number, $i = x, y, z$), a is the lattice constant of cubic crystal, $\overline{u^2}$ is the mean square of the thermal displacement of an atom from the equilibrium position. The last quantity is calculated in the frame of Debye model of the lattice oscillations [18,27–29]. Following Ter-Mikaelyan [18] (who solved this problem for static BrS of relativistic electron scattered by monocrystal) the channel described by the first term in the right-hand side of equality (3) we have named the incoherent channel, and the another one corresponding to the second term in (3) we have named the coherent channel. With the help of formulae (1)–(3) one can see that each of these channels is divided into static and polarization ones.

In the case of coherent channel besides the energy conservation law (which naturally holds also for incoherent channel) there is the quasi-momentum conservation law described by Dirac delta-function in formula (3):

$$E_i - E_f = \omega, \qquad \mathbf{p}_i - \mathbf{p}_f = \mathbf{k} + \mathbf{g}. \qquad (4)$$

Using formulae (1)–(3) one can obtain the expression for doubly differential cross section $d\sigma/d\omega\, d\Omega$ when the angle between the direction of radiation and momentum vector $\mathbf{p}_i$ is equal to 90°. This cross section describes the BrS from the polycrystalline target. It is derived by an averaging of microcrystal cross section among all possible microcrystal orientations. It is suggested in this averaging that all orientations have the equal probability [8].

BrS cross section per one target atom in polycrystalline medium multiplied by photon energy within the frame of dipole approximation is given by the following expressions:

$$\frac{\omega\, d\sigma}{d\omega\, d\Omega} = \frac{\alpha r_e^2 c^2 Z^2}{4\pi v_i^2}(I_1 + I_2),$$

$$I_1 = \int\limits_{1-\sqrt{1-\beta}}^{1+\sqrt{1-\beta}} \frac{d\mathbf{q}}{\mathbf{q}^3}\left(1 - e^{-q^2 b}\right) \times \left[\beta^2 + 4\left(1 + \frac{\beta}{2}\right)\mathbf{q}^2 + \mathbf{q}^4\right],$$

$$\mathbf{q} = \frac{\mathbf{p}_i - \mathbf{p}_f}{\mathbf{p}_i}, \qquad b = 4\pi^2\frac{\overline{u^2}}{\lambda_i^2}, \qquad \beta = \frac{\hbar\omega}{E_i},$$

$$I_2 = \frac{1}{4\pi}\sum_{\mathbf{g}_0}\frac{|S(\mathbf{g})|^2}{\mathbf{g}_0^3}\left(1 + \cos^2\vartheta_{\mathbf{g}}\right)e^{-g^2\overline{u^2}} \times \Theta(1 - \cos\vartheta_{\mathbf{g}}),$$

$$\cos\vartheta_{\mathbf{g}} = \frac{a}{\lambda}\frac{c}{v_i}\frac{1}{\mathbf{g}_0} + \frac{\mathbf{g}_0}{2}\frac{\lambda_i}{a}. \qquad (5)$$

Here α is the fine structure constant, r_e is the classical radius of electron, c is the speed of light, v_i and λ_i are the velocity and de Broglie wavelength of incident electron, Z is the atomic number of the target's element. Integration in I_1 is performed with respect to dimensionless transferred momentum $\mathbf{q}$. Summation in I_2 is made over all possible values of vector $\mathbf{g}_0$, where $\mathbf{g}_0$ is dimensionless vector of reciprocal lattice: $\mathbf{g} = (2\pi/a)\mathbf{g}_0$. The value $\mathbf{g}_0 = 0$ should be excluded from the sum because in the case of $\mathbf{g}_0 = 0$ the conservation laws (4) cannot be simultaneously satisfied. $\vartheta_{\mathbf{g}}$ is the angle between vector $\mathbf{p}_i$ and $\mathbf{g}$. Expression for $\cos\vartheta_{\mathbf{g}}$ can be derived from the conservation laws (4) in the frame of dipole approximation with respect to wavelength $\lambda = 2\pi c/\omega$. Heaviside Θ-function in formulae (5) provides the simultaneous satisfaction of the conservation laws (4). One can see from the expression for $\cos\vartheta_{\mathbf{g}}$ that the sum over $\mathbf{g}_0$ is finite. Formulae (5) are given in the Gauss system of units.

Two approximations simplifying the calculations are used in the derivation of formulae (5). These are the high-frequency approximation for atomic polarizability and approximation of "stripped" nucleus. Amplitude of PBrS contains the atomic polarizability that is defined by the sum over virtual transitions between ground atomic state and all other atomic states. In the case when the photon energy exceeds energies of all essential virtual transition the sum for polarizability is reduced and can be expressed via atomic form-factor [11]. If, moreover, the dipole approximation with respect to wavelength λ is correct then atomic form-factor describing screening in the static amplitude and form-factor originating from the atomic polarizability mutually annihilate and the total BrS is reduced to static BrS on "stripped" nucleus. Undoubted use of the calculations made in [16] consists particularly in the determination of the applicability limits for the "stripped" nucleus approximation.

Let us consider the physical sense of the formulae (5). The first term in the right-hand side of (5) describes the transfer of the momentum from the incident electron to the target via incoherent channel. The second term describes the transfer of the momentum via coherent channel. In the second case the BrS process takes place in the periodic field of all lattice atoms. Therefore, the quasi-momentum conservation law must be satisfied. In this case the change of the projectile momentum is determined by the discrete multitude of the reciprocal lattice vectors and therefore momentum transfer occurs by only discrete portions.

The analogous situation takes place in the X-ray scattering by the crystalline targets. Then the first channel corresponds to the diffusion scattering and the second channel corresponds to the diffraction one [28]. The exponential factors in I_1 and I_2 are the Debye–Waller factors. Such factor also arises in the X-ray scattering theory [28] and in the theory of the Mössbauer effect [29].

The results of our numerical calculations are presented in Fig. 1 for polycrystalline silver target (face-centered cubic lattice, $a = 4.09$ Å, $\sqrt{\overline{u^2}} = 0.087$ Å for room temperature). Curves "1" and "2" in this figure describe the total and incoherent BrS in the "stripped" nucleus approximation, i.e., with the polarization effect. One can see that when the coherent channel is "switched on" then the characteristic saw-like curve describing the BrS spectrum arises. The positions of maxima and steps of this saw-like curve correspond to the discrete switching on new values of $\mathbf{g}$ vectors in the I_2 sum with decreasing of the frequency ω, i.e., these

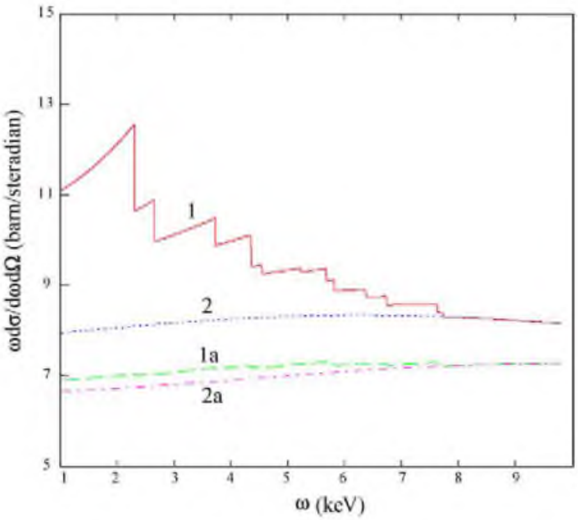

Fig. 1. Differential cross section of bremsstrahlung of non-relativistic electron of the energy 50 keV scattered in the polycrystalline silver. Cross section is calculated with respect to one target atom and multiplied on the photon energy with and without polarization channel. Ordinate is in barn/steradian. Angle between vector $\mathbf{p}_i$ and vector $\boldsymbol{\kappa}$ is equal to $90°$. Solid line—two channels are taken into account: coherent and incoherent and polarization effect; dotted line—only incoherent channel is taken into account with polarization effect; dashed line—two channels are taken into account without polarization effect; dashed-dotted line—only incoherent channel is taken into account without polarization effect (within the framework of exponential screening).

positions connect with the quasi-momentum conservation laws (4).

Curves 1a and 2a are the same as the curves 1 and 2 except for the substantial difference that 1a and 2a were calculated for the static amplitude in (1) only. Corresponding formulae can be obtained from (5) if one inserts the factor $|Z - F(\mathbf{q})|^2$ under the integral sign in I_1 instead of the factor Z^2 and the factor $|Z - F(\mathbf{g})|^2$ should be inserted under the summation sign in I_2. In our calculations we used the exponential model for the screening of atomic nucleus. In this model the electrostatic field of an atom is described with the help of Yukawa potential [18]. The factor $|Z - F(\mathbf{g})|^2$ strongly depresses the "saw-likeness" of the spectrum of static BrS because it is small for small $\mathbf{g}$ values which give the main contribution into the coherent cross section. Terms in I_2 decrease with the increase of $\mathbf{g}$ value and so a few terms (with small $\mathbf{g}$) play the main role. In our calculations we restrict by the first 12 terms. It should be noted that although the oscillations of saw-like curve depend on the calculation model the fact of its existence and the positions of its steps and maxima are determined by the conservation laws only.

In the summary we compare our results with BH theory. Let formally $\overline{u^2} = \infty$ for the absolute temperature $T \to \infty$. Then the contribution of the coherent channel disappears for disappears the exponent describing the thermal vibrations of atoms in the expression for the incoherent channel. If moreover only the static term in the formula (1) is preserved then the expression (5) is reduced to BH formula. In this case the transition from gas to solid state comes to the increase of the atomic concentration only. In another limiting case when $T \to 0$ the coherent channel strongly dominates over the incoherent one although $\overline{u^2}$ is not equal to zero because of the vacuum atomic oscillations.

Thus, in the calculations of BrS of non-relativistic electron scattered by polycrystalline target we account for the new substantial factors: thermal oscillations of atoms, periodicity of the crystalline medium and polarization effect. Experiments for the discovering of the saw-like character of the BrS spectrum from polycrystalline targets should account for the non-monochromaticity of the electron beam, angle size of the photodetector, real crystalline structure of the target and its temperature. It is interesting to find out the possibilities of the modulation methods application in this problem (for instance, one can use the deformation oscillations of the solid target to measure the dependence of the BrS spectrum on the modulation of the lattice constant).

Although our final formulae relate to the polycrystalline targets used in many BrS experiments the conclusion on the essentiality of solid-state effects in BrS is true also for monocrystals [30].

Progress in the BrS measurements achieved in the recent work [17] provides the hope that the influence of the polycrystalline structure on the BrS of non-relativistic electron will be found.

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