

## Coherent bremsstrahlung in imperfect periodic atomic structures

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Coherent bremsstrahlung of high energy electrons moving in a three-dimensional imperfect periodic lattice consisting of a complicated system of atoms is considered. On the basis of the normalized probability density function of the distribution of atomic centers in the fundamental cell the relations describing coherent and incoherent contributions into cross sections are obtained. In particular, the cross section of coherent bremsstrahlung in complex polyatomic single crystals is found. The peculiarities of formation and possibilities of utilization of coherent processes are discussed.

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### I. INTRODUCTION

For the first time, the theory of the coherent bremsstrahlung and electron-positron pair production in single crystals was published in Refs. 1–3. Up to now, these processes have been much studied both theoretically<sup>4–6</sup> and experimentally.<sup>7–9</sup> The specific peculiarities of the coherent processes were widely used for obtaining linearly polarized  $\gamma$  beams in polarization measurements<sup>10–12</sup> and for increasing the  $e^\pm$ -beam intensity.<sup>13</sup> These experimental investigations were carried out in a wide energy range of electron, positron and  $\gamma$  beams from a few hundreds of MeV to 100–200 GeV. As a rule, simple crystallographic structures were used in experiments. Both experiments and theory show that, with the increasing of the particle energy, the requirements on the beam divergence become more strict. Besides, at high enough energies the process of coherent bremsstrahlung is violated, due to the magneto-bremsstrahlung mechanism.<sup>6</sup> This mechanism provides the linear polarization of the emitted  $\gamma$  quanta. However, a sufficiently small angle divergence of the electron beam is needed for utilizing this phenomenon. One of the main requirements, which restricts the use of coherent processes, is the small size of the fundamental cell of the single crystals, which has to be of the order of some angstroms. It is our opinion that, finding atomic periodic structures with a minimal period of tens or hundreds angstroms, may yield a good solution to the above-mentioned problem.

In recent years, considerable advances have been made in the creation of various nanostructures,<sup>14–16</sup> such as regular two-dimensional arrays, fullerite crystals, nanofilms, nanotube superlattices and so on. In a number of papers<sup>17–19</sup> nanotube lattices were considered as a source of channeling radiation. Other applications of nanotubes for purposes of high energy physics are also described in Refs. 20–22.

According to Ref. 14 single-wall nanotubes are uniform in diameter and self-organized into ropes, which consist of 100 to 500 nanotubes in a two-dimensional triangular lattice with a lattice constant of 17 angstroms. In our talk<sup>20</sup> we discussed the processes of coherent bremsstrahlung and  $e^\pm$ -pair production in the nanotube superlattice. In considering this task we met problems, the solution of which has a common meaning for the above-mentioned coherent pro-

cesses in various nanostructures and complex single crystals. Below we give an introduction to these problems, using the example of the nanotube superlattice.

Figure 1 illustrates the three-dimensional superlattice of (10,10) armchair single wall nanotubes. In this case we can write for the vector-radius  $\mathbf{r}_j(x_j, y_j, z_j)$  of the  $j$ th atom in the nanotube,

$$x_{1,j} = R \cos\left(\frac{4\pi j}{N} + \varphi_1\right), \quad x_{2,j} = R \cos\left(\frac{4\pi j}{N} + \varphi_2\right), \quad (1)$$

$$y_{1,j} = R \sin\left(\frac{4\pi j}{N} + \varphi_1\right), \quad y_{2,j} = R \sin\left(\frac{4\pi j}{N} + \varphi_2\right), \quad (2)$$

$$z_{1,j} = 0, \quad z_{2,j} = b/2, \quad (3)$$

where  $j = 1, 2, \dots, N/2$  are the indices corresponding to atoms placed in two parallel planes,  $R$  is the radius of the ring,  $b$  is the period (i.e., the size of the fundamental cell) in the  $z$  direction, and  $\varphi_1, \varphi_2$  are the angle shifts ( $\varphi_1 - \varphi_2 = \text{const}$ ).

In Fig. 1 we describe an ideal nanostructure where the angle shifts of all nanotubes are the same. The experiments<sup>14</sup> show that these angle shifts are distributed randomly or, in other words, every nanotube is turned at some different angle. This means that the content of every cell will be different, relative to the coordinate system. Thus, the nanotube lattice is not a periodic structure in a strict sense, in spite of the constancy of the distance between neighboring nanotubes. However, the existing theory of coherent bremsstrahlung holds its validity for atomic structures (single crystals), which are periodic in a strict sense.

Based on this example, we formulate the common problem for the calculation of the coherent bremsstrahlung in artificial and natural nanostructures. The problem is the violation of the periodicity in a strict sense in these structures.

This situation is well known in the diffraction physics of x rays<sup>23</sup> in imperfect structures. However, the process of coherent bremsstrahlung was investigated and utilized mainly in simple single crystals. Such crystals as silicon and diamond have a negligibly small degree of mosaicity and admixture. Because of this fact, the problem of calculation of the bremsstrahlung in imperfect structures did not practically

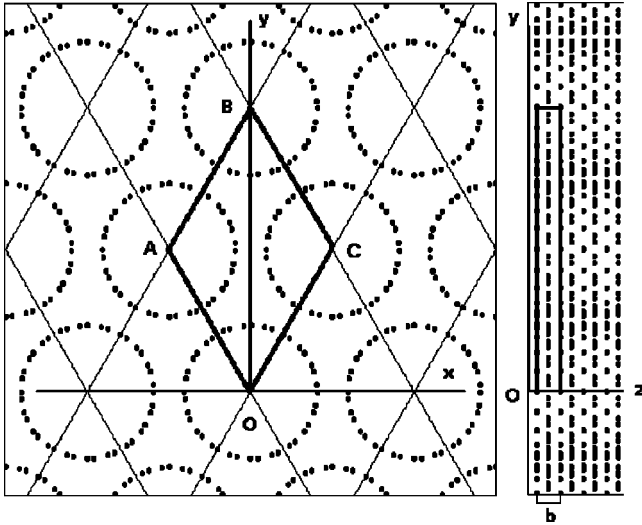


FIG. 1. The three-dimensional superlattice of (10,10) armchair single-wall nanotubes and Cartesian coordinate system ( $xyz$ ). The fundamental cell of the structure is presented with the help of the thick lines. The black points are atoms of the nanotubes.  $OA=AB=BC=CO=17 \text{ \AA}$ ,  $b=2.4 \text{ \AA}$ , radius of circles  $R=6.8 \text{ \AA}$ .

appear (except for the problem of the thermal atomic motion<sup>2</sup>). In the x-ray diffraction theory the above-mentioned problem was solved with the help of the introduction of the averaged electron density.<sup>23</sup> In our talk,<sup>20</sup> using the analogy in the description of the diffraction and coherent processes, we could solve this problem on the basis of a physical sense. Besides, we suggest another approach which is based on computer simulations. We think that this approach may be extended to a wide class of analogous problems, in particular, for a nanotube lattice with a more complicated dependence on the angle shifts, than a random one.

It turns out that our computer approach has an analytical solution in the general case. Furthermore, on the basis of our method we are able to consider the process of coherent bremsstrahlung in imperfect atomic structures, taking into account all fluctuation factors.

The paper is organized as follows. In sect. II we give a mathematical introduction to the problem. In Sect. III, for the description of fluctuations in atomic structures, we introduce the normalized probability density function and formulate some rules for averaging the structure factors. In sect. IV we consider the three-dimensional model of the real atomic structure with fluctuations. The results obtained here allow us to derive (in Sect. V) the coherent and incoherent cross sections of the bremsstrahlung process in imperfect structures. In sec. VI we discuss the influence of thermal fluctuations in atomic structures on the coherent bremsstrahlung. Here we reproduce well known results and also obtain new ones. In sec. VII we consider the possibility of generalizing our theory to consider multiatomic structures and, in particular, multiatomic single crystals. Samples of calculations of the bremsstrahlung process in real atomic structures are presented in Sec. VIII. In conclusion (in sec. IX) we give shortly the main results of our investigations.

## II. CROSS SECTION OF COHERENT BREMSSTRAHLUNG IN IDEAL PERIODIC STRUCTURES

The differential cross section of the coherent bremsstrahlung for an ideal periodic structure, consisting of atoms, can be written in the following form:<sup>2</sup>

$$d\sigma_{CB} = d\sigma_{BG} \left| \sum_i e^{i\mathbf{q}\mathbf{r}_{i0}/\hbar} \right|^2, \quad (4)$$

where  $\sigma_{BG}$  is the bremsstrahlung cross section for an isolated atom,  $\mathbf{q}$  is the three-dimensional transfer momentum, and  $\mathbf{r}_{i0}$  are the vector radii of the atoms in the periodic structure.

From this expression, the following relation for the cross section per atom<sup>2</sup> is derived:

$$d\sigma_{CB}(E, E_\gamma, \mathbf{q}) = \frac{(2\pi)^3}{NV} \sum_{\mathbf{g}} d\sigma_{BG}(E, E_\gamma, \mathbf{q}) |S(\mathbf{g})|^2 \delta(\mathbf{q}/\hbar - \mathbf{g}), \quad (5)$$

where  $N$  is the number of atoms in the fundamental cell of the structure,  $V$  is the volume of the fundamental cell,  $S(\mathbf{g})$  is the structure factor,<sup>2,4</sup>  $\mathbf{g}$  is the vector of the reciprocal lattice,  $\delta$  is the delta function,  $E, E_\gamma$  are the energies of the initial electron and bremsstrahlung  $\gamma$  quantum and  $\hbar$  is the Planck constant. The structure factors are calculated from the relation

$$S(\mathbf{g}) = \sum_{j=1}^N e^{i\mathbf{g}\mathbf{r}_j}, \quad (6)$$

where  $\mathbf{r}_j$  is the radius of the  $j$ th atom in the fundamental cell.

From Eq. (5) one can see that the specific character of every atomic structure is defined by its structure factors. It is obvious that for ideal structures (at a fixed localization of the atoms) the structure factors take well defined values. Because of various fluctuations, the coordinates of atoms in the fundamental cell are changed with space and (or) time and this fact does not allow us to use Eq. (5) for calculations. For this reason, it is necessary to understand the behavior of the structure factors for these fluctuations.

The plan of our further actions for solving the above-mentioned problem is the following: we will try to reduce the problem to one, for which the solution is known (such as the process in the ideal periodic lattice). In the first stage of the study, we will formulate the definition and some rules for the averaged structure factors. Then, we will consider the simulations of fluctuations on the model of real periodic structures, and thereafter we will use the obtained results for the calculation of the coherent bremsstrahlung cross section in imperfect atomic structures.

It should be noted that in the theory of coherent bremsstrahlung the potential of the crystal is considered as the sum of isolated atomic potentials. It is obvious that this assumption is only approximately true. However, the current experimental experience (see, for example, Ref. 4) shows the correctness of this statement with a high enough accuracy. In this paper we will also hold this statement true and because of this, our results will be easy to compare with the standard theory. In the following, we will make use of the expression

“coordinates of the atomic center” which has an exact physical meaning denoting the coordinates of the atomic nucleus.

### III. AVERAGING OF THE STRUCTURE FACTORS

As previously noted, the specific character of every structure is defined by its structure factors. It is useful to appreciate the physical meaning of these quantities. For this purpose, we write the atomic density for a periodic structure in the point given by the vector radius  $\mathbf{r}$ ,

$$n_a(\mathbf{r}) = \sum_k \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_k - \mathbf{r}_j) = \frac{N}{V} + \frac{1}{V} \sum_{\mathbf{g}} S(\mathbf{g}) e^{-i\mathbf{g}\mathbf{r}}. \quad (7)$$

From here, it follows that  $S(\mathbf{g})/V$  is the Fourier component of the atomic density or, in other words, the structure factors are the atomic images in the reciprocal space. Note that Eq. (7) does not take into account thermal atomic fluctuations. They are easy to calculate with the help of the following multiplier:  $\exp(-A\mathbf{g}^2/2)$  (see below). We stress that the structure factors depend on the choice of a coordinate system and therefore the values of structure factors have a physical meaning only in a defined coordinate system.

The space distribution of the atomic centers in the fundamental cell of the structure can be described with the help of the normalized probability density function  $\mathcal{P}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ , where  $\mathbf{x}_1, \dots, \mathbf{x}_N$  are the space displacements of the atomic centers from the points  $\mathbf{r}_j$  in the cell. The integral of this function over the whole ( $3 \times N$ -dimensional)  $\mathcal{V}$  volume of the cell is equal to 1. Then the structure factor, averaged with the help of the  $\mathcal{P}$  function, is given by

$$\begin{aligned} \langle S(\mathbf{g}) \rangle &= \int S(\mathbf{g}, \mathbf{r}_1 - \mathbf{x}_1, \dots, \mathbf{r}_N - \mathbf{x}_N) \mathcal{P}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathcal{V} \\ &= \sum_{j=1}^N e^{i\mathbf{r}_j \mathbf{g}} \int_V e^{-i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j, \end{aligned} \quad (8)$$

where the  $\mathcal{F}_j$  function reads as

$$\mathcal{F}_j(\mathbf{x}_j) = \int \mathcal{P} d\mathcal{V}(-j), \quad (9)$$

with  $d\mathcal{V}(-j) = d\mathbf{x}_1 d\mathbf{x}_2 \dots d\mathbf{x}_{j-1} d\mathbf{x}_{j+1} \dots d\mathbf{x}_N$ . Now we can find the following coordinate-independent value:

$$\begin{aligned} \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle &= \sum_{j=1}^N \int_V e^{-i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j \int_V e^{i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j \\ &+ \sum_{i,j=1, i \neq j}^N e^{i(\mathbf{r}_i - \mathbf{r}_j) \mathbf{g}} \int_V e^{i(\mathbf{x}_j - \mathbf{x}_i) \mathbf{g}} \mathcal{F}_i(\mathbf{x}_i) \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_i d\mathbf{x}_j. \end{aligned} \quad (10)$$

In a similar manner, one can define the average square module of the structure factor,

$$\begin{aligned} \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle &= \int S(\mathbf{g}, \mathbf{r}_1 - \mathbf{x}_1, \dots, \mathbf{r}_N - \mathbf{x}_N) \\ &\times S^*(\mathbf{g}, \mathbf{r}_1 - \mathbf{x}_1, \dots, \mathbf{r}_N - \mathbf{x}_N) \mathcal{P}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathcal{V} \\ &= N + \sum_{i,j=1, i \neq j}^N e^{i(\mathbf{r}_i - \mathbf{r}_j) \mathbf{g}} \\ &\times \int_V e^{-i(\mathbf{x}_i - \mathbf{x}_j) \mathbf{g}} \mathcal{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j) d\mathbf{x}_i d\mathbf{x}_j, \end{aligned} \quad (11)$$

where

$$\mathcal{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j) = \int \mathcal{P} d\mathcal{V}(-i, -j). \quad (12)$$

Here the term  $d\mathcal{V}(-i, -j)$  indicates that the integration takes place over all space variables, except the ones belonging to the  $i, j$  atoms. Taking into account the relations obtained here, we can write for the dispersion

$$\begin{aligned} \langle \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle \rangle &= N - \sum_{j=1}^N \int_V e^{-i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j \int_V e^{i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j \\ &+ \sum_{i,j=1, i \neq j}^N e^{i(\mathbf{r}_i - \mathbf{r}_j) \mathbf{g}} \int_V e^{-i(\mathbf{x}_i - \mathbf{x}_j) \mathbf{g}} [\mathcal{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j) \\ &- \mathcal{F}_i(\mathbf{x}_i) \mathcal{F}_j(\mathbf{x}_j)] d\mathbf{x}_i d\mathbf{x}_j, \end{aligned} \quad (13)$$

where we introduced the following notation:  $\langle \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle \rangle = \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle - \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle$ .

In the case when the  $x_i$  and  $x_j$  variables are statistically independent, the following relation takes place:  $\mathcal{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j) = \mathcal{F}_i(\mathbf{x}_i) \mathcal{F}_j(\mathbf{x}_j)$ . If all  $N$  atoms are statistically independent, the normalized probability density function may be represented as  $\mathcal{P} = \prod_{j=1}^N \mathcal{F}_j(\mathbf{x}_j)$  and Eq. (13) can be rewritten in the following form:

$$\langle \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle \rangle = N - \sum_{j=1}^N \int_V e^{-i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j \int_V e^{i\mathbf{x}_j \mathbf{g}} \mathcal{F}_j(\mathbf{x}_j) d\mathbf{x}_j. \quad (14)$$

In the case when all the atoms in the fundamental cell are equivalent, this equation has the following simple form:

$$\langle \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle \rangle = N(1 - \langle s(\mathbf{g}) \rangle \langle s^*(\mathbf{g}) \rangle), \quad (15)$$

where  $\langle s \rangle$  is the averaged function,

$$\langle s(\mathbf{g}) \rangle = e^{i\mathbf{r}\mathbf{g}} \int_V e^{-i\mathbf{x}\mathbf{g}} \mathcal{F}(\mathbf{x}) d\mathbf{x}. \quad (16)$$

It should be noted that, for an ideal atomic structure,  $\mathcal{F}_j(\mathbf{x}_j) = \delta(\mathbf{x}_j)$  for every  $j$  and then  $\langle \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle \rangle = 0$ .

It is significant that the equations in this section are valid for any vector  $\mathbf{g}$  of the reciprocal space, in particular for any vector of the reciprocal lattice. Besides, there are no indications of the atomic sorts in the equations. Below, it will be shown that the cross section of the coherent bremsstrahlung depends on the averaged structure factors for monoatomic structures and on some combinations of similar factors for

multiatomic structures. Thus, Eqs. (8)–(16) are also useful in the case of structures consisting of different atoms.

#### IV. SIMULATION OF FLUCTUATIONS

Let us build the three-dimensional ( $\mathcal{N} \times \mathcal{N} \times \mathcal{N}$ ) cubic lattice consisting of identical cubic cells with side size equal to  $a$ . Then we can put into every cell an identical number of atoms, which we denote by  $N$ . Doing this, it would mean knowing the coordinates of every atoms in every cell. Let us select a local Cartesian coordinate system in every cell. Besides, the probability function of localization of atoms in the cell will be considered as known  $\mathcal{P}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ . Let us suppose that the atomic coordinates in every cell are distributed according to this function.

To be specific, we select the basic Cartesian coordinate system in the left and bottom corner of the lattice. With this lattice (of  $\mathcal{N}a \times \mathcal{N}a \times \mathcal{N}a$  size) as the basic element, we can build (by using parallel translations in  $x, y, z$  directions with a period of  $\mathcal{N}a$ ) the three-dimensional infinite periodic (in the strict sense) structure. The main idea in our consideration stems from the fact that the above described superlattice (at large enough  $N$ ) contains practically all combinations of atoms in the small cells (according to the normalized probability density function  $\mathcal{P}$ ) and, on the other hand, this superlattice is periodic in a strict sense. Thus, we can use the coherent bremsstrahlung theory for describing the radiation processes. For this purpose, the structure factors of the large lattice should be found for every reciprocal vector  $\tilde{\mathbf{g}}$ . Further we will introduce an overtilde above the values relative to the large cube lattice with the side of  $\mathcal{N}a$ . Thus, these structure factors  $\tilde{S}$  can be calculated from the following relation:

$$\tilde{S}(\tilde{\mathbf{g}}) = \sum_{i=1}^{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} e^{i\tilde{\mathbf{g}}\mathbf{r}_{ijk}} S_{ijk}(\tilde{\mathbf{g}}), \quad (17)$$

where the reciprocal vector  $\tilde{\mathbf{g}}$  is

$$\tilde{\mathbf{g}} = G_0 l \mathbf{e}_x + G_0 m \mathbf{e}_y + G_0 n \mathbf{e}_z, \quad l, m, n = 0, \pm 1, \pm 2, \dots \quad (18)$$

Here  $G_0 = 2\pi/(\mathcal{N}a)$ ,  $\mathbf{e}_x$ ,  $\mathbf{e}_y$  and  $\mathbf{e}_z$  are the unit vectors in  $x, y, z$  directions and the translation vector reads as  $\mathbf{r}_{ijk} = (i-1)a\mathbf{e}_x + (j-1)a\mathbf{e}_y + (k-1)a\mathbf{e}_z$  in the basic coordinate system. In Eq. (17),  $S_{ijk}(\tilde{\mathbf{g}})$  denotes the following structure factor:  $\sum_{\alpha=1}^N \exp i\tilde{\mathbf{g}}\mathbf{r}_{ijk\alpha}$ , where  $\mathbf{r}_{ijk\alpha}$  is the vector radius of the  $\alpha$ th atom in the local coordinate system of the  $ijk$  cell. The multiplication  $\tilde{\mathbf{g}}\mathbf{r}_{ijk}$  reads as

$$\tilde{\mathbf{g}}\mathbf{r}_{ijk} = 2\pi \left( \frac{l(i-1)}{\mathcal{N}} + \frac{m(j-1)}{\mathcal{N}} + \frac{n(k-1)}{\mathcal{N}} \right). \quad (19)$$

For large enough numbers  $\mathcal{N}$  one can find

$$\tilde{S}(\tilde{\mathbf{g}}) = \sum_{i=1}^{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} S_{ijk}(\tilde{\mathbf{g}}) \approx \mathcal{N}^3 \langle S(\tilde{\mathbf{g}}) \rangle, \quad (20)$$

where  $\langle S(\tilde{\mathbf{g}}) \rangle$  is the structure factor  $S_{ijk}$  averaged over the coordinates and the quantities  $l/\mathcal{N}, m/\mathcal{N}, n/\mathcal{N}$  are integer numbers. In the other cases, one can write

$$\tilde{S}(\tilde{\mathbf{g}}) \rightarrow 0, \quad \text{at } \mathcal{N} \rightarrow \infty. \quad (21)$$

Equation (20) is obvious, so at the pointed condition the value  $\tilde{\mathbf{g}}\mathbf{r}_{ijk}$  is multiplied by  $2\pi$  and the exponents in Eq. (20) are equal to 1. For obtaining Eq. (21) we should take into account that there is only a finite number of the various exponents in Eq. (17) (this number  $N_{\text{exp}} \leq \mathcal{N}$ , the equality holding when  $\mathcal{N}$  is a prime number). Grouping the terms near the same exponents, we get

$$\tilde{S}(\tilde{\mathbf{g}}) = \sum_{p=1}^{N_{\text{exp}}} \left( e^{2\pi p/N_{\text{exp}}} \sum S_{ip} \right) \approx \sum S_{ip} \sum_{p=1}^{N_{\text{exp}}} e^{2\pi p/N_{\text{exp}}} = 0. \quad (22)$$

Here we can remove  $\sum S_{ip}$  terms, due to their approximated equality at large enough  $\mathcal{N}$ .

We can consider the structure factor  $\tilde{S}(\tilde{\mathbf{g}})$  as a statistical variable. Taking into account Eqs. (20) and (21), we find that  $\langle \tilde{S}(\tilde{\mathbf{g}}) \rangle = \mathcal{N}^3 \langle S(\tilde{\mathbf{g}}) \rangle$  when  $l/\mathcal{N}, m/\mathcal{N}, n/\mathcal{N}$  are simultaneously integer numbers and  $\langle \tilde{S}(\tilde{\mathbf{g}}) \rangle = 0$  in the other cases.

Similar calculations allow us to obtain the averaged dispersion of the structure factor  $\tilde{S}(\tilde{\mathbf{g}})$  for the case of large  $\mathcal{N}$  numbers

$$\langle \langle \tilde{S}(\tilde{\mathbf{g}}) \tilde{S}^*(\tilde{\mathbf{g}}) \rangle \rangle = \mathcal{N}^6 \langle \langle S(\tilde{\mathbf{g}}) S^*(\tilde{\mathbf{g}}) \rangle \rangle. \quad (23)$$

This equation is valid for arbitrary  $l, m, n$  numbers. However, the value  $\tilde{S}$  is defined by the limit of Eq. (20) in the case when  $l/\mathcal{N}, m/\mathcal{N}, n/\mathcal{N}$  are integer numbers, and  $\langle \tilde{S} \rangle = 0$  in the other cases (see Eq. (21)).

It should be noted that our previous consideration is based on the specific kind of the crystallographic structure. It is easy to verify that our analysis is valid in the general case. Indeed, the important relation for the correctness of the theory (see Eq. (19)) is valid for any real crystallographic structure.<sup>24,25</sup> Of course, in the general case, the vector of the reciprocal lattice and the translation vector must be written in the corresponding (generally nonorthogonal) coordinate system.

#### V. CROSS SECTION

In principle, now we can calculate the coherent bremsstrahlung cross section for the structure described in the previous section. However, we call to the attention of the reader the fact that the structure factors  $\tilde{S}$ , in the case when the  $l/\mathcal{N}, m/\mathcal{N}, n/\mathcal{N}$  numbers are nonintegral ones, tend to zero at large  $\mathcal{N}$ . Nevertheless, the contribution from these factors to the calculated values may be noticeable, due to their large amount.

In this case, the differential cross section of coherent bremsstrahlung has the following form:

$$d\sigma_{CB} = \frac{(2\pi)^3}{\mathcal{N}^3 \tilde{V}} \sum_{\tilde{\mathbf{g}}} d\sigma_{BG} \tilde{S}(\tilde{\mathbf{g}}) \tilde{S}^*(\tilde{\mathbf{g}}) \delta(\mathbf{q}/\hbar - \tilde{\mathbf{g}}). \quad (24)$$

Here  $\tilde{V} = \mathcal{N}^3 V$  is the volume of the fundamental cell of the structure.



When the number  $\mathcal{N}$  is large enough, we can write (see Eqs. (20)–(23))

$$\tilde{S}(\tilde{\mathbf{g}})\tilde{S}^*(\tilde{\mathbf{g}}) \approx \langle \tilde{S}(\tilde{\mathbf{g}})\tilde{S}^*(\tilde{\mathbf{g}}) \rangle = \langle \tilde{S}(\tilde{\mathbf{g}}) \rangle \langle \tilde{S}^*(\tilde{\mathbf{g}}) \rangle + \mathcal{N}^3 \langle \langle S(\tilde{\mathbf{g}})S^*(\tilde{\mathbf{g}}) \rangle \rangle \quad (25)$$

for the case of the simultaneously integer numbers  $l/\mathcal{N}, m/\mathcal{N}, n/\mathcal{N}$  and

$$\tilde{S}(\tilde{\mathbf{g}})\tilde{S}^*(\tilde{\mathbf{g}}) \approx \langle \tilde{S}(\tilde{\mathbf{g}})\tilde{S}^*(\tilde{\mathbf{g}}) \rangle = \mathcal{N}^3 \langle \langle S(\tilde{\mathbf{g}})S^*(\tilde{\mathbf{g}}) \rangle \rangle \quad (26)$$

for the other cases. Taking into account these relations and Eq. (20), we get

$$d\sigma_{CB} = \frac{(2\pi)^3}{NV} \sum_{\mathbf{g}} d\sigma_{BG} \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle \delta(\mathbf{q}/\hbar - \mathbf{g}) + \frac{(2\pi)^3}{N\tilde{V}} \sum_{\tilde{\mathbf{g}}} d\sigma_{BG} \langle \langle S(\tilde{\mathbf{g}})S^*(\tilde{\mathbf{g}}) \rangle \rangle \delta(\mathbf{q}/\hbar - \tilde{\mathbf{g}}). \quad (27)$$

We see that the total cross section represents the sum of two terms. We interpret the first term as the averaged coherent contribution. Indeed, the value of this cross section calculated per atom is proportional to  $N$  and inversely proportional to  $V$ . In addition, this cross section is independent of  $\mathcal{N}$ , which defines the size of the large lattice.

It is obvious that the second term describes the common effect due to the incoherent bremsstrahlung in the  $\mathcal{N} \times \mathcal{N} \times \mathcal{N}$  lattice at large  $\mathcal{N}$  values and the coherent one in the infinite superlattice. Now we can find the energetic cross section by integration over  $\mathbf{q}$ ,

$$d\sigma_{CB} = dE_{\gamma} \left\{ \int_{\mathbf{q}_m}^{\infty} \frac{(2\pi)^3}{NV} \sum_{\mathbf{g}} d\sigma_{BG} \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle \delta(\mathbf{q}/\hbar - \mathbf{g}) d\mathbf{q} + \frac{(2\pi\hbar)^3}{N\tilde{V}} \sum_{\tilde{\mathbf{g}}} d\sigma_{BG}(E, E_{\gamma}, \hbar\tilde{\mathbf{g}}) \langle \langle S(\tilde{\mathbf{g}})S^*(\tilde{\mathbf{g}}) \rangle \rangle \right\}, \quad (28)$$

where  $\mathbf{q}_m$  is the vector directed along the velocity of the electron beam and  $q_m = \hbar\delta + q_{\perp}^2 c/E$ ,  $q_{\perp}$  is the transversal projection of  $\mathbf{q}$  on the primary electron direction of motion,  $m$  is the electron mass,  $c$  is the speed of light, and for the minimal value of the transfer momentum  $\hbar\delta$  we use the traditional notation.

We see that the second term in Eq. (28) is proportional to a sum over reciprocal vectors  $\tilde{\mathbf{g}}$  (see Eq. (18)). At large  $N$ , this sum is most conveniently expressed by an integral representation. For this purpose, we use the relation  $dl dm dn = d\tilde{\mathbf{g}}/G_0^3 = d\mathbf{q}/(\hbar G_0^3)$ . As a result, we get

$$d\sigma_{CB} = dE_{\gamma} \left\{ \int_{\mathbf{q}_m}^{\infty} \frac{(2\pi)^3}{NV} \sum_{\mathbf{g}} d\sigma_{BG} \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle \delta(\mathbf{q}/\hbar - \mathbf{g}) d\mathbf{q} + \frac{1}{N} \int_{\mathbf{q}_m}^{\infty} d\sigma_{BG} \langle \langle S(\mathbf{q})S^*(\mathbf{q}) \rangle \rangle d\mathbf{q} \right\}. \quad (29)$$

We stress that the structure factors in the first term (see Eq. (29)) are discrete values, which depend on the reciprocal lattice vectors  $\mathbf{g}$ , and that the structure factor  $S(\mathbf{q})$  in the second term is a continuous function of the  $q/\hbar$  variable. Note that passing from a discrete to a continuous description,

one removes the action of the large periodic lattice.

Thus, in principle, we have solved the problem of the coherent bremsstrahlung in imperfect periodic atomic structures. In fact, Eq. (29) represents the sum of the coherent and incoherent contributions in the cross section:  $d\sigma_{BC} = d\sigma_c + d\sigma_i$ . Now both cross sections should be reduced to a form which is convenient for specific calculations.

First of all, we find the coherent contribution. For this purpose, it is necessary to simplify the cross section  $d\sigma_{BG}$  as it was described in Ref. 2. This simplification is based on the fact that the effective range of  $q \ll mc$ , due to thermal fluctuations.

Using this condition, and with the help of calculations similar to those in Refs. 2,4, we can obtain for the coherent cross section

$$x \frac{d\sigma_c}{dx} = \sigma_0 \left[ (1 + (1-x)^2) \psi_1 - \frac{2}{3}(1-x) \psi_2 \right], \quad (30)$$

where  $\sigma_0 = \alpha_{QED} Z^2 r_e^2$ ,  $\alpha_{QED} = 1/137.04$ ,  $r_e$  is the classical electron radius,  $x = E_{\gamma}/E$  is the ratio of the emitted photon energy  $E_{\gamma}$  to the initial energy  $E$  of the electron, and  $\psi_1, \psi_2$  functions are

$$\psi_1 = 4 \frac{(2\pi)^2}{NV} \sum_{\mathbf{g}} |U(\mathbf{g})|^2 \frac{\delta g_{\perp}^2}{g_{\parallel}^2}, \quad (31)$$

$$\psi_2 = 24 \frac{(2\pi)^2}{NV} \sum_{\mathbf{g}} |U(\mathbf{g})|^2 \frac{\delta^2 g_{\perp}^2 (g_{\parallel} - \delta)}{g_{\parallel}^4}. \quad (32)$$

Here  $\mathbf{g}$  is the vector of the reciprocal lattice,  $g_{\parallel}$  is the projection of the  $\mathbf{g}$  vector on the direction of the particle motion,  $g_{\perp}^2 = g^2 - g_{\parallel}^2$ , and the  $\hbar\delta$  value is given by

$$\hbar\delta = \frac{m^2 c^3}{2E} \frac{x}{1-x}. \quad (33)$$

The summation in Eqs. (31) and (32) is carried out under the following condition:

$$g_{\parallel} \geq \delta. \quad (34)$$

The  $|U(\mathbf{g})|^2$  values are

$$|U(\mathbf{g})|^2 = \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle \frac{(1 - F(\mathbf{g}))^2}{g^4}, \quad (35)$$

where  $F(\mathbf{g})$  is the atomic form factor. These equations differ from the standard theory by the averaged structure factor in Eq. (35).

Next, we simplify the second integral in Eq. (29) describing the incoherent contribution. From Eq. (14) we see that the incoherent cross section may be represented as the difference  $(d\sigma_{BG} - d\sigma_d)$ , where  $d\sigma_{BG}$  is the cross section for the process of bremsstrahlung in the corresponding amorphous media and  $d\sigma_d$  is the cross section depending on the averaged structure factors. This allows us to simplify Eq. (29),

$$x \frac{d\sigma_i}{dx} = \sigma_0 \left[ (1 + (1-x)^2) \psi_{1s}^i - \frac{2}{3}(1-x) \psi_{2s}^i \right], \quad (36)$$

where the functions  $\psi_{1s}^i, \psi_{2s}^i$  have the following form:

$$\psi_{1s}^{\mu} = \psi_{1BG}^{\mu} - \psi_{1d}^{\mu}, \psi_{2s}^{\mu} = \psi_{2BG}^{\mu} - \psi_{2d}^{\mu}. \quad (37)$$

$$\psi_{1d}^{\mu} = \frac{2\hbar\delta}{N} \int_0^{\infty} dq_{\perp}^2 \int_{\hbar\delta}^{\sim mc} [\langle\langle S(\mathbf{q})S^*(\mathbf{q}) \rangle\rangle - N] \times \frac{[1-F(q)]^2 q_{\perp}^2}{q^4} dq_{\parallel}, \quad (38)$$

$$\psi_{2d}^{\mu} = \frac{12(\hbar\delta)^2}{N} \int_0^{\infty} dq_{\perp}^2 \int_{\hbar\delta}^{\sim mc} [\langle\langle S(\mathbf{q})S^*(\mathbf{q}) \rangle\rangle - N] \times \frac{[1-F(q)]^2 q_{\perp}^2 (q_{\parallel} - \hbar\delta)}{q^4} dq_{\parallel}, \quad (39)$$

and the well-known<sup>2,4</sup> functions  $\psi_{1BG}^{\mu}$  and  $\psi_{2BG}^{\mu}$  are

$$\psi_{1BG}^{\mu}(\delta) = 4 + 4 \int_{\hbar\delta}^{\sim mc} (q - \hbar\delta)^2 \frac{[1-F(q)]^2}{q^3} dq, \quad (40)$$

$$\psi_{2BG}^{\mu}(\delta) = 10/3 + 4 \int_{\hbar\delta}^{\sim mc} \left( q^3 - 6\hbar^2 \delta^2 q \ln\left(\frac{q}{\hbar\delta}\right) + 3\hbar^2 \delta^2 q - 4\hbar^3 \delta^3 \right) \frac{[1-F(q)]^2}{q^4} dq. \quad (41)$$

Equations (38) and (39) were obtained under the assumption that  $q \ll mc$ , which is always valid for real atomic structures. In the case when the  $S$  factors are functions only of the  $q$  variable, Eqs. (38) and (39) are simplified,

$$\psi_{1d}^{\mu} = 4 \int_{\hbar\delta}^{\sim mc} (q - \hbar\delta)^2 [\langle\langle S(q)S^*(q) \rangle\rangle / N - 1] \frac{[1-F(q)]^2}{q^3} dq, \quad (42)$$

$$\psi_{2d}^{\mu} = 4 \int_{\hbar\delta}^{\sim mc} \left( q^3 - 6\hbar^2 \delta^2 q \ln\left(\frac{q}{\hbar\delta}\right) + 3\hbar^2 \delta^2 q - 4\hbar^3 \delta^3 \right) \times [\langle\langle S(q)S^*(q) \rangle\rangle / N - 1] \frac{[1-F(q)]^2}{q^4} dq. \quad (43)$$

When the condition of complete screening is fulfilled, Eqs. (40) and (41) take the following simple form:

$$\psi_{1BG}^{\mu} = 4 \ln 183Z^{-1/3}, \quad \psi_{2BG}^{\mu} = 4 \ln 183Z^{-1/3} - 2/3. \quad (44)$$

Note that the cross section  $d\sigma_{BC}$  can be found in another way with the help of the Fourier transform (see Ref. 2). However, this method is longer and requires straightforward but cumbersome calculations.

## VI. AVERAGING OVER THERMAL FLUCTUATIONS

The relations obtained in this paper describe the process of coherent bremsstrahlung in imperfect periodic structures. One can see that, in the general case, the cross section is the sum of coherent and incoherent contributions. Thermal atomic fluctuations always take place in atomic structures.

Let us apply our theory for the study of their influence on the coherent bremsstrahlung spectrum. Here we take into account the simplest case, when the thermal fluctuations are isotropic in space and independent of the location of other atoms. Then, in accordance with Refs. 2,6,

$$\mathcal{F}_j(\mathbf{x}_j) = \frac{\exp(-x_j^2/(2A))}{(2\pi A)^{3/2}}, \quad (45)$$

and  $\mathcal{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j) = \mathcal{F}_i(\mathbf{x}_i)\mathcal{F}_j(\mathbf{x}_j)$ . The normalized probability density function is equal to the product of all  $\mathcal{F}_j$  functions. From Eqs. (8)–(16) we find

$$\langle S(\mathbf{g}) \rangle = \sum_{j=1}^N e^{i\mathbf{r}_j \mathbf{g}} e^{-A\mathbf{g}^2/2} = S(\mathbf{g}) e^{-A\mathbf{g}^2/2}, \quad (46)$$

$$\langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle = S(\mathbf{g}) S^*(\mathbf{g}) e^{-A\mathbf{g}^2}, \quad (47)$$

$$\langle\langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle\rangle = N(1 - e^{-A\mathbf{g}^2}). \quad (48)$$

In order to take into account these fluctuations, we need to substitute  $\langle S \rangle$  and  $\langle S S^* \rangle$  values in Eqs. (35), (42), and (43). In this case the relations for the incoherent part of the cross section are in agreement with similar ones in Refs. 2–4 and 6.

One can assume that in most cases the mechanism violating the ideal structure acts independently of the thermal fluctuations. Then the normalized probability density function  $\mathcal{P}$  of the structure may be written in the following form:  $\mathcal{P}(\mathbf{r}_1, \dots, \mathbf{r}_N, \mathbf{r}_1^T, \dots, \mathbf{r}_N^T) = \mathcal{P}_C(\mathbf{r}_1, \dots, \mathbf{r}_N) \mathcal{P}_T(\mathbf{r}_1^T, \dots, \mathbf{r}_N^T)$ , where  $\mathcal{P}_T$  is the normalized probability density function for thermal fluctuations (see Eq. (46)), and  $\mathcal{P}_C$  is some other similar function. Let us consider the case when the atomic system is described by Eq. (46), or, in other words, we assume that all atoms in the fundamental cell are equivalent, with respect to thermal fluctuations. Then, we get

$$\langle S \rangle_{TC} = e^{-A\mathbf{g}^2/2} \langle S \rangle_C, \quad (49)$$

$$\langle\langle S S^* \rangle\rangle_{TC} = N - (N - \langle\langle S S^* \rangle\rangle_C) e^{-A\mathbf{g}^2}, \quad (50)$$

where the symbols  $T$  and  $C$  denote the corresponding averaging. Under a similar assumption, that all atoms in the cell are equivalent, we get, instead of Eq. (50),

$$\langle\langle S S^* \rangle\rangle_{TC} = N(1 - e^{-A\mathbf{g}^2} \langle s \rangle \langle s^* \rangle). \quad (51)$$

The equations obtained here may be substituted into Eqs. (35), (42), and (43) and the problem of calculating the coherent bremsstrahlung for atomic systems, with the conditions pointed out above, is solved.

## VII. COHERENT BREMSSTRAHLUNG IN DIATOMIC SINGLE CRYSTALS

It is well known that the process of coherent bremsstrahlung may be considered as a result of the electron motion in a continuous periodic potential.<sup>6</sup> In the case of imperfect periodic structures, we can also write the effective averaged potential,

$$\varphi(\mathbf{r}) = \frac{4\pi eZ}{V} \sum_{\mathbf{g}} \langle S(\mathbf{g}) \rangle \frac{(1-F(\mathbf{g}))}{g^2} e^{-i\mathbf{g}\mathbf{r}}, \quad (52)$$

where  $\langle S(\mathbf{g}) \rangle$  is the averaged structure factor. From Eq. (52) one can also get one- and two-dimensional potentials (see Refs. 6,26).

As it can be seen from Eq. (52), our consideration is valid for monoatomic single crystals. However, the case of the

polyatomic periodic structure may be studied in a similar manner. Let us consider the diatomic perfect periodic structure. We can represent this structure as the sum of two independent structures, one of them consisting of atoms with  $Z_1$  number, and the other consisting of atoms with  $Z_2$  number. Both structures have the same periods and the crystallographic type of the three-dimensional lattice. We can write the three-dimensional potential for this structure as

$$\varphi(\mathbf{r}) = \frac{4\pi e}{V} \sum_{\mathbf{g}} \frac{[Z_1 S(\mathbf{Z}_1, \mathbf{g})(1-F(\mathbf{Z}_1, \mathbf{g})) + Z_2 S(\mathbf{Z}_2, \mathbf{g})(1-F(\mathbf{Z}_2, \mathbf{g}))]}{g^2} e^{-i\mathbf{g}\mathbf{r}}, \quad (53)$$

where  $F(\mathbf{Z}_1, \mathbf{g}), F(\mathbf{Z}_2, \mathbf{g})$  are the corresponding atomic form factors and  $S(\mathbf{Z}_1, \mathbf{g}), S(\mathbf{Z}_2, \mathbf{g})$  are the structure factors for every sublattice. They have a form as in Eq. (6):  $S(\mathbf{Z}_1, \mathbf{g}) = \sum_{j=1}^{N_1} \exp i\mathbf{r}_j \mathbf{g}$ ,  $S(\mathbf{Z}_2, \mathbf{g}) = \sum_{j=1}^{N_2} \exp i\mathbf{r}_j \mathbf{g}$ , but the sum should be taken separately over atoms of each sort, these numbers being denoted as  $N_1, N_2$ . The total number of atoms in the fundamental cell is equal to  $N=N_1+N_2$ .

Then, we should take into account that the bremsstrahlung scattering amplitude is proportional to the Fourier transform of the potential (see Eq. (53)) and the cross section is proportional to the squared amplitude. Thus, we can get the cross section of the process in the perfect periodic structure, which is defined by the following factor:

$$Y(\mathbf{Z}_1, \mathbf{Z}_2, \mathbf{g}) = [Z_1 S(\mathbf{Z}_1, \mathbf{g})(1-F(\mathbf{Z}_1, \mathbf{g})) + Z_2 S(\mathbf{Z}_2, \mathbf{g})(1-F(\mathbf{Z}_2, \mathbf{g}))]. \quad (54)$$

The coherent bremsstrahlung cross section is proportional to the  $YY^*$  value.

With the help of the above-considered method one can get the corresponding cross section for the imperfect periodic diatomic structures. In the general case, the function  $\mathcal{P}$  contains the space variables for every atom in the fundamental cell, and different correlations between various atoms are possible, in principle. Below, we will write the final result for coherent bremsstrahlung in the diatomic structures, taking into account thermal fluctuations. We carry out our calculations, under the assumption that fluctuations of all atoms are isotropic and independent, but the squared radius of the vibrations depends on the sort of atoms. The final result for the cross section, calculated per fundamental cell, has the following form:

$$x \frac{d\sigma}{dx} = \alpha_{QED} r_e^2 \left[ (1 + (1-x)^2)(\psi_1 + \psi_1^f) - \frac{2}{3}(1-x)(\psi_2 + \psi_2^f) \right], \quad (55)$$

where

$$\psi_1 = 4 \frac{(2\pi)^2}{V} \sum_{\mathbf{g}} \langle Y(\mathbf{g}) \rangle \langle Y^*(\mathbf{g}) \rangle \frac{\delta g_{\perp}^2}{g^4 g_{\parallel}^2}, \quad (56)$$

$$\psi_2 = 24 \frac{(2\pi)^2}{V} \sum_{\mathbf{g}} \langle Y(\mathbf{g}) \rangle \langle Y^*(\mathbf{g}) \rangle \frac{\delta^2 g_{\perp}^2 (g_{\parallel} - \delta)}{g^4 g_{\parallel}^4}. \quad (57)$$

The summation in Eqs. (56) and (57) is carried out with the condition  $g_{\parallel} \geq \delta$ . The functions  $\psi_1^f, \psi_2^f$  are calculated according to

$$\psi_{1d}^f = N_1 Z_1^2 \psi_{1BG}(Z_1)^a + N_2 Z_2^2 \psi_{1BG}(Z_2) - \psi_{1d}^f, \quad (58)$$

$$\psi_{2d}^f = N_1 Z_1^2 \psi_{2BG}(Z_1)^a + N_2 Z_2^2 \psi_{2BG}(Z_2) - \psi_{2d}^f, \quad (59)$$

where

$$\psi_{1d}^f = 4 \int_{\hbar\delta}^{\sim mc} (q - \hbar\delta)^2 [\langle Y(q) Y^*(q) \rangle - N_1 Z_1^2 (1-F(\mathbf{Z}_1))^2 - N_2 Z_2^2 (1-F(\mathbf{Z}_2))^2] \frac{dq}{q^3}, \quad (60)$$

$$\psi_{2d}^f = 4 \int_{\hbar\delta}^{\sim mc} \left( q^3 - 6\hbar^2 \delta^2 q \ln \left( \frac{q}{\hbar\delta} \right) + 3\hbar^2 \delta^2 q - 4\hbar^3 \delta^3 \right) \times [\langle Y(q) Y^*(q) \rangle - N_1 Z_1^2 (1-F(\mathbf{Z}_1))^2 - N_2 Z_2^2 (1-F(\mathbf{Z}_2))^2] \frac{dq}{q^4}, \quad (61)$$

with  $\langle Y(q) Y^*(q) \rangle = \langle Y(q) Y^*(q) \rangle - \langle Y(q) \rangle \langle Y^*(q) \rangle$ .

In the case of thermal fluctuations, one can find

$$\langle Y(\mathbf{g}) \rangle = Z_1 S(\mathbf{Z}_1, \mathbf{g})(1-F(\mathbf{Z}_1, \mathbf{g})) e^{-A_1 g^2/2} + Z_2 S(\mathbf{Z}_2, \mathbf{g})(1-F(\mathbf{Z}_2, \mathbf{g})) e^{-A_2 g^2/2}, \quad (62)$$

$$\langle Y(\mathbf{g}) Y^*(\mathbf{g}) \rangle = N_1 Z_1^2 (1-F(\mathbf{Z}_1, \mathbf{g}))^2 (1 - e^{-A_1 g^2}) + N_2 Z_2^2 (1-F(\mathbf{Z}_2, \mathbf{g}))^2 (1 - e^{-A_2 g^2}), \quad (63)$$

where  $A_1$  and  $A_2$  are the squared radii of the thermal vibrations, for the first and second sorts of atoms, respectively. We recall that, in Eqs. (62) and (63), the variable  $\mathbf{g}$  is discrete in the calculation of the coherent contribution and continuous for the incoherent one.

In a similar manner one can calculate the cross section for periodic structures consisting of three and more atoms. Note that the total intensity radiation per unit of length in multi-atomic structures may be calculated as  $N_c E \int_0^1 x(d\sigma/dx)dx$ , where  $d\sigma/dx$  is defined by Eq. (55) and  $N_c = 1/V$  is the number of fundamental cells per unit volume.

## VIII. EXAMPLES OF CALCULATIONS

### A. Limiting cases of atomic structures

Let us consider an ideal atomic structure. Obviously, the  $\mathcal{P}$  function for this structure is given by the following multiplication:

$$\mathcal{P}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \prod_{j=1}^N \delta(\mathbf{x}_j). \quad (64)$$

Taking this fact into account, we get  $\langle S(\mathbf{g})S^*(\mathbf{g}) \rangle - \langle S(\mathbf{g}) \rangle \langle S^*(\mathbf{g}) \rangle = 0$ . This means that, for an ideal atomic structure, the incoherent contribution in the cross section is equal to zero.

Now we consider a monoatomic homogeneous amorphous medium. We can find the mean volume  $V = a^3$  per atom and build the cubic fundamental cell, which contains  $N$  atoms. This means that the cube side of this cell is equal to  $N^{1/3}a$ . We take the  $\mathcal{P}$  function as a product of the following functions defined on the whole volume of the fundamental cell:

$$\mathcal{P} = \prod_{j=1}^N \mathcal{F}_j(\mathbf{x}_j), \quad \mathcal{F}_j(\mathbf{x}_j) = \frac{1}{8b^3}, \quad -b \leq x_{ji} \leq b, \quad (65)$$

$$i = 1, 2, 3, \quad b = N^{1/3}a/2.$$

The averaged structure factor (see Eq. (16)) for an atom in the cell is

$$\langle s(\mathbf{q}) \rangle = 8 \frac{\sin(N^{1/3}aq_1/2)\sin(N^{1/3}aq_2/2)\sin(N^{1/3}aq_3/2)}{Na^3q_1q_2q_3}. \quad (66)$$

In general, we consider the variable  $\mathbf{q}$  in the latter equation as a continuous one. However, for the calculation of the coherent contribution, we should take a discrete set of quantities of the variable, which is described by a relation similar to Eq. (18). Substituting in Eq. (66)  $q_j = \frac{4\pi}{b}l_j$  ( $l_j = 1, 2, 3, \dots$ ) we get  $\langle s(\mathbf{q}) \rangle = 0$ , and according to Eq. (8) every discrete structure factor  $S$  is also equal to 0. This means that there is no coherent contribution in the cross section.

Taking into account the calculations of the incoherent contribution, we should consider the  $\langle s(\mathbf{q}) \rangle$  value as a function of the continuous variable  $\mathbf{q}$ . It is easy to see that the  $\langle s(\mathbf{q}) \rangle \langle s^*(\mathbf{q}) \rangle$  value at small  $\mathbf{q}$  is approximately equal to 1 and at large enough  $\mathbf{q}$  this value is significantly less than 1. The larger are the numbers  $N$ , and then the smaller are the  $q$  values at which this rule holds. Taking into account that there exists a minimum transfer momentum in the bremsstrahlung process, we can select the value of  $N$  such that

$\langle s(\mathbf{q}) \rangle \langle s^*(\mathbf{q}) \rangle \approx 0$ , and therefore  $\langle \langle S(\mathbf{q})S^*(\mathbf{q}) \rangle \rangle \approx N$ . In this case the incoherent contribution is the same as in the corresponding amorphous medium. With the help of a similar function (see Eq. (65)) one can describe the transition from a three-dimensional structure to two-dimensional or one-dimensional ones.

### B. Nanotube superlattice

Let us calculate the bremsstrahlung cross section in the nanotube superlattice (see Fig. 1 and Eqs. (1)–(3)), under the assumption of a random distribution of the angle shifts. In this case we rewrite Eqs. (1)–(3) in cylindrical coordinates  $\rho, \varphi, z$ ,

$$\rho_{1,j} = R, \quad \rho_{2,j} = R, \quad (67)$$

$$\varphi_{1,j} = \varphi_{1,1} + 4\pi(j-1)/N, \quad \varphi_{2,j} = \varphi_{2,1} + 4\pi(j-1)/N, \quad (68)$$

$$z_{1,j} = 0, \quad z_{2,j} = b/2, \quad (69)$$

where  $j = 1, \dots, N/2$  and  $\varphi_{1,1} - \varphi_{2,1} = \text{const}$ . These equations describe the various nanotubes. In particular, for a (10, 10) armchair single nanotube, we have  $N = 40$ ,  $\varphi_{1,1} - \varphi_{2,1} = 4\pi/(3N)$  and the other geometric parameters are shown in Fig. 1.

It is easy to see that the problem of averaging has only one independent coordinate,  $\varphi_{1,1}$ , for instance. In principle, for its solution one can get the necessary averaging values with the simple density function  $1/2\pi$ . However, for the sake of illustration, we begin with giving the  $\mathcal{P}$  function,

$$\mathcal{P} = \frac{1}{2\pi} \delta(z_{1,1}) \frac{\delta(\rho_{1,1} - R)}{R} \prod_{j=2}^{N/2} \delta\left(\varphi_{1,j} - \varphi_{1,1} - \frac{4\pi}{N}(j-1)\right) \times \frac{\delta(z_{1,j}) \delta(\rho_{1,j} - R)}{R} \prod_{j=1}^{N/2} \delta\left(\varphi_{2,j} - \varphi_{2,1} - \frac{4\pi}{N}(j-1)\right) \times \frac{\delta(z_{2,j} - b/2) \delta(\rho_{2,j} - R)}{R}, \quad (70)$$

with the unit of volume

$$d\mathcal{V} = \prod_{j=1}^{N/2} \rho_{1,j} d\rho_{1,j} d\varphi_{1,j} dz_{1,j} \prod_{j=1}^{N/2} \rho_{2,j} d\rho_{2,j} d\varphi_{2,j} dz_{2,j}. \quad (71)$$

From this we find the  $\mathcal{F}_{ij}$  functions,

$$\mathcal{F}_{[m,i],[n,j]} = \frac{1}{2\pi} \delta\left(\varphi_{n,j} - \varphi_{m,i} + \frac{4\pi}{N}(i-j) + \Delta_{n,m}\right) \times \frac{\delta(z_{n,j} - b_{n,m}) \delta(\rho_{n,j} - R)}{R} \frac{\delta(z_{m,i} - b_{n,m}) \delta(\rho_{m,i} - R)}{R}. \quad (72)$$

Here every atom is labeled by a pair of numbers  $m, i$ , where  $m = 1$  or  $2$  is the number of the ring (see Fig. 1) and  $i = 1, 2, \dots, N/2$  is the atomic number in the selected ring. The



value  $\Delta_{n,m}$  is equal to  $\varphi_{1,1}-\varphi_{2,1}=\Delta_{2,1}=-\Delta_{1,2}$  when  $n \neq m$ , and it vanishes when  $n=m$ , and the value is equal to 0 or  $b/2$ , in accordance with Eq. (70).

From here, we can obtain by integration

$$\mathcal{F}_{[m,i]} = \frac{1}{2\pi} \frac{\delta(z_{m,i} - b_{n,m}) \delta(\rho_{m,i} - R)}{R}. \quad (73)$$

Now we can calculate the averaged structure factors

$$\langle S(g_{\perp}, g_z) \rangle = \frac{N}{2} J_0(Rg_{\perp}) (1 + e^{ibg_z/2}). \quad (74)$$

Here  $J_0(x)$  is the Bessel function of the zeroth order and  $g_{\perp}, g_z$  are the values of the reciprocal vector projection on the  $xy$  plane and its projection on the  $z$  axis, respectively (see Fig. 1). Equation (74) describes the continuous structure factors. For the determination of the discrete set of the structure factors, needed for calculating the coherent contribution (see Eqs. (30)–(35)), it is necessary to substitute in Eq. (74) the projections of the reciprocal vectors  $\mathbf{g}_{\perp} = (2\pi/a)((l-m)\mathbf{e}_x + (l+m)\mathbf{e}_y/\sqrt{3})$ ,  $g_z = (2\pi/b)n\mathbf{e}_z$  for the triangular crystallographic lattice. As a result, we get  $S(l, m, n) = NJ_0(Rg_{\perp})$  for even  $n$  numbers and 0 for odd ones.

Then we find

$$\begin{aligned} \langle \langle S(\mathbf{g}) S^*(\mathbf{g}) \rangle \rangle &= 2 \sum_{\nu=1}^{N/2} \sum_{\eta=1}^{N/2} \left[ J_0 \left( 2g_{\perp} R \sin \left( \frac{4\pi}{N} (\nu - \eta) \right) \right) \right. \\ &+ J_0 \left( 2g_{\perp} R \sin \left( \frac{4\pi}{N} (\nu - \eta) + (\varphi_2 - \varphi_1) \right) \right) \cos(g_z b/2) \left. \right] \\ &- N^2 J_0^2(g_{\perp} R) (1 + \cos(g_z b/2))/2. \end{aligned} \quad (75)$$

From these equations one can see that the obtained averaged structure factors are functions of the  $q_{\perp}$  and  $q_z$  variables. This means that it is necessary to use Eqs. (38) and (39) in the calculations. We compute first the internal integral, which is given by

$$I(q, \hbar\delta) = \int_0^{q^2 - (\hbar\delta)^2} \frac{\langle \langle S(\mathbf{q}) S^*(\mathbf{q}) \rangle \rangle / (N-1) q_{\perp}^2 dq_{\perp}^2}{(q^2 - q_{\perp}^2)^{3/2}}. \quad (76)$$

One can see that the region  $q^2 - q_{\perp}^2 \sim (\hbar\delta)^2$  gives the main contribution (for  $b\delta \ll 1$ ). Thus, we can replace the value  $q_{\perp}$  by  $q$  in Eqs. (38) and (39), and then we can also use Eqs. (42) and (43).

Figure 2 illustrates the structure factors for an ideal (10, 10) single wall nanotube superlattice, and for this lattice with the random distribution of angle shifts. One can see that the values of the structure factors are smaller, in the latter case, at large enough  $q$  quantities. However, the first few factors are the same, in between.

Figure 3 illustrates the behavior of the  $\langle \langle S(\mathbf{q}) S^*(\mathbf{q}) \rangle \rangle$  value as a function of the transferred momentum. The thin curve describes this function, according to Eq. (75), and the thick one describes this, as a result of averaging over thermal fluctuations (see also Eq. (49)). The smooth curve of middle thickness represents the behavior of the function

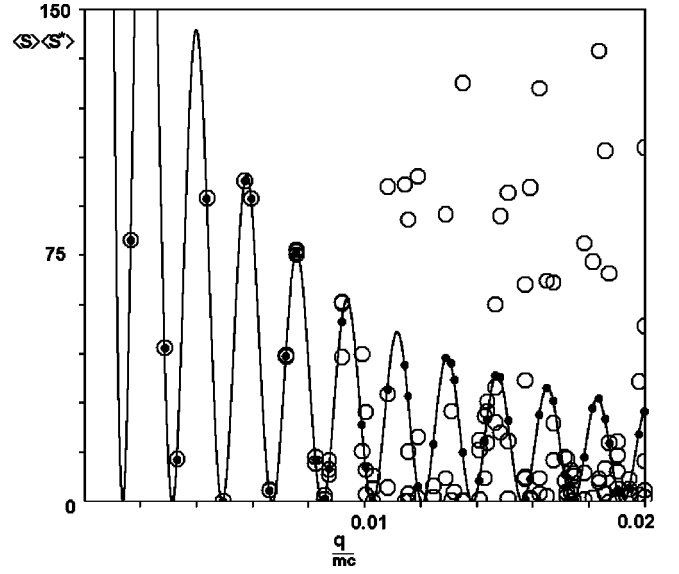


FIG. 2. Structure factors for the superlattice of (10,10) armchair single-wall nanotubes as a function of the transferred momentum  $q$  (in  $mc$  units). The circles present the ideal structure and the black points present the structure with the random distribution of the angle shifts. The curve is the function  $N^2 J_0^2(qR)$ .

$N(1 - \exp(-Ag^2))$ . One can see that all the above pointed functions tend to  $N$ , at large enough  $q$  values.

Now we can calculate the incoherent cross section of the investigated process. For this purpose, we find the functions  $\psi_{1s}^l$  and  $\psi_{2s}^l$  (see Fig. 4). One can see that these functions are slightly smaller than for an amorphous medium. It should be noted that the calculations were carried out for a three-dimensional structure of nanotubes. Our estimate shows that, for a two-dimensional nanotube lattice, the incoherent contribution is practically the same as in an amorphous medium.

The differential intensity of the coherent bremsstrahlung is shown in Fig. 5.

### C. Scheelite structures

In this section we consider the coherent bremsstrahlung in three-atomic single crystals of the scheelite type. For specific calculations, we select  $\text{PbWO}_4$  and  $\text{CaWO}_4$  single crystals. It is interesting to notice that  $\text{PbWO}_4$  single crystals are widely used for the realization of electromagnetic calorimeters.<sup>27</sup> In Ref. 28 it was shown that the coherent radiation in such structures influences some characteristics of the calorimeters.

A crystallographic structure of the scheelite type is shown in Fig. 6. The fundamental cell is represented by a tetragonal prism with the side of the squared basis and the height which are equal to 5.44 (5.22) and 12.01 (11.45) angstroms for the  $\text{PbWO}_4$  ( $\text{CaWO}_4$ ) single crystal, respectively. The fundamental cell contains 4 lead (calcium), 4 tungsten and 16 oxygen atoms. The oxygen atoms are located at the corners of the tetragons around the tungsten atoms.

Using relations similar to Eqs. (55)–(61) we have calculated the differential intensity ( $x d\sigma_{CB}/dx$ ) and the linear polarization of coherent bremsstrahlung in  $\text{PbWO}_4$  and  $\text{CaWO}_4$  single crystals. In these calculations we use three different

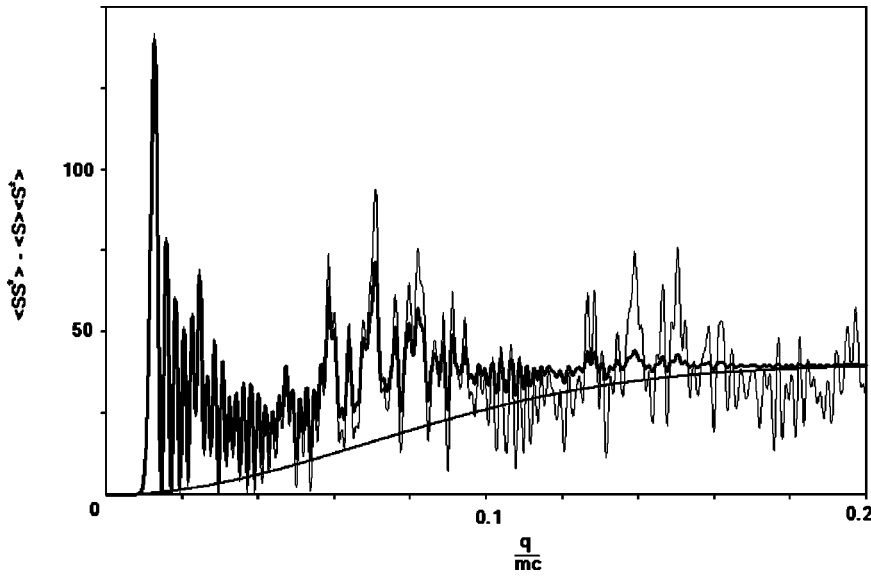


FIG. 3. The behavior of  $\langle\langle S(\mathbf{q})S^*(\mathbf{q}) \rangle\rangle$  as a function of the transferred momentum in  $mc$  units (see explanations in the text).

amplitudes of thermal fluctuations. One can expect that the energy of the fluctuations is the same for every sort of atom.<sup>24</sup> This means that the amplitude of fluctuations is inversely proportional to the atomic mass. For tungsten atoms we select an amplitude equal to 0.04 angstroms (as in the tungsten single crystal at room temperature). Note that the intensity of the coherent radiation depends weakly enough on the amplitude of fluctuations, and hence our approach is justified.

The calculations were carried out for the case when the electron momentum lies in the  $yz$  plane (see Figs. 7 and 8) and the angle between the  $z$  axis and the direction of motion is equal to 5 mrad. One can see that the behavior of the curves is different for both single crystals. Note that the difference in the lattice constants of both single crystals is small

and, because of this, it cannot yield the explanation of the effect. For an understanding of the effect, we should take into account that in monoatomic structures the values of the structure factors determine the set of allowed points of the reciprocal lattice. In our case, the  $\langle Y \rangle \langle Y^* \rangle$  values play an analogous role. The different behavior of these values for the two different single crystals is the main issue in the description of coherent processes. So, the coherent bremsstrahlung in a  $\text{PbWO}_4$  single crystal is similar to this process in a monoatomic single crystal. Indeed, the contribution in the intensity of oxygen atoms is small, due to the low  $Z$  value. For the tungsten and lead atoms, the form factors and

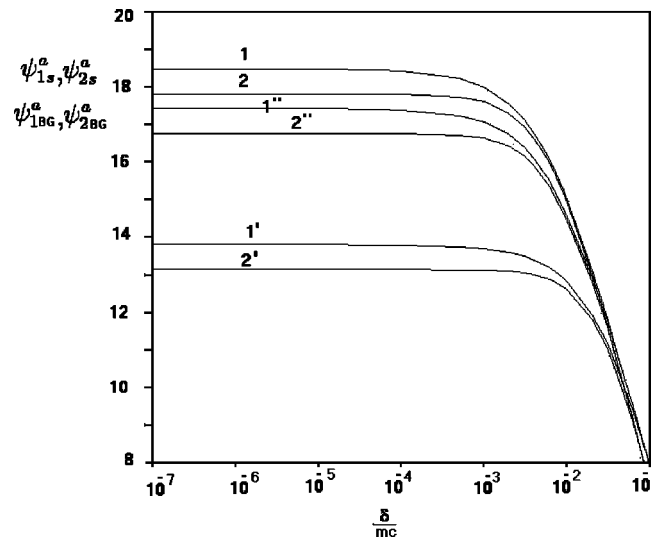


FIG. 4. Dependence of the functions  $\psi_{1BG}^a, \psi_{2BG}^a$  (1,2) and  $\psi_{1s}^a, \psi_{2s}^a$  on the minimal transfer momentum (in  $mc$  units). The curves 1', 2' represent the result of averaging over thermal fluctuations, and the curves 1'', 2'' represent the total result of averaging over both thermal fluctuations and angle shifts.

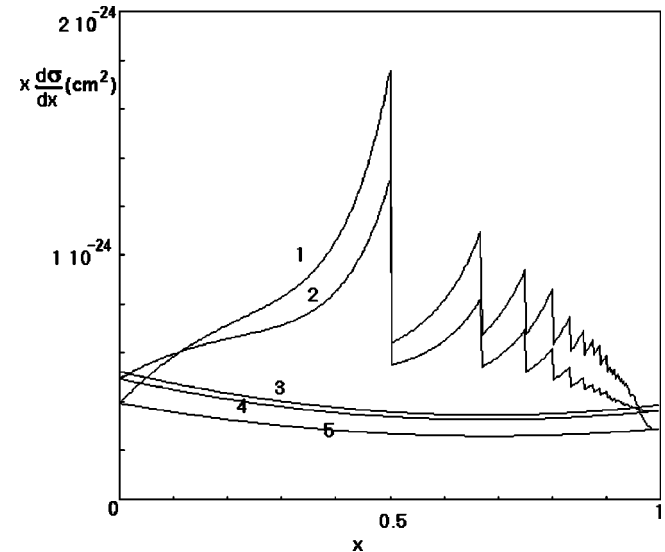


FIG. 5. Differential photon spectra in the (10,10) armchair single wall nanotube superlattice for the structure at fixed angle  $\varphi_{1,1}=0$  (1) and for one with random angle shift distribution (2). The electron energy is equal to 10 GeV. The electron beam moves in the  $(xz)$  plane (see Fig. 1) under 0.018 rad with respect to the  $z$  axis. Curves 3, 4, 5 illustrate the incoherent contribution for conditions corresponding to the cases (1,2), (1', 2'), (1'', 2'') (see Fig. 4), respectively.

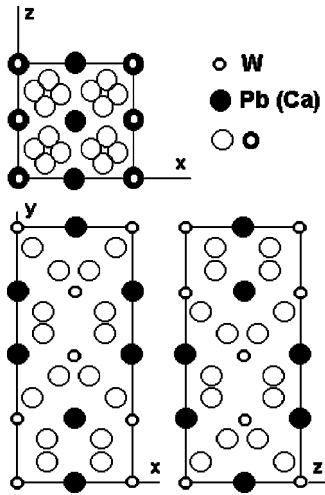


FIG. 6. Three projections of atoms in the fundamental cell of the scheelite crystallographic structure.

charges are approximately equal in between, and the allowed points are approximately defined with the help of the factor  $\sigma_{j=1}^8 \exp(-\mathbf{g}\mathbf{r}_j)$ .

The degree of linear polarization can be defined from the relations

$$P(x) = \frac{2(1-x)\alpha_{QED}r_e^2\psi_3(\delta)}{x d\sigma(x)/dx}, \quad (77)$$

$$\psi_3(\delta) = \frac{4(2\pi)^2\delta^3}{V} \sum_{\mathbf{g}} \langle Y \rangle \times \langle Y^* \rangle \frac{(g_x^2 - g_y^2)\cos(2\beta) + 2g_x g_y \sin(2\beta)}{g^4 g_{\parallel}^4}, \quad (78)$$

where  $g_x, g_y$  are the components of the  $\mathbf{g}$  vector on the  $x$  and  $y$  axes and  $\beta$  is the angle between the  $yz$  plane and the arbitrary plane where the  $z$  axis is located.<sup>4</sup> Figures 7 and 8 illustrate also the degree of linear polarization. The maximal polarization takes place when in Eq. (77) the incoherent contribution is significantly less than the coherent one. This situation may be realized for high energy values of the electron beam.

#### D. Some remarks

It is necessary to point out the specific peculiarities of coherent bremsstrahlung, which apply to our examples. The intensities of coherent radiation obtained in this paper were calculated for special orientations of the atomic structures, and they represent so-called ideal spectra.<sup>4</sup> Due to the specific motion of electrons in the atomic structures, for the description of the real spectra we need to take into account the additional intensity of radiation arising from the nearby directions of motion. This additional intensity takes place mainly for small  $x$  values. However, the above mentioned orientations are convenient for comparison, in various conditions of the radiation sources (such as different orientations or atomic structures), and they are widely covered in the

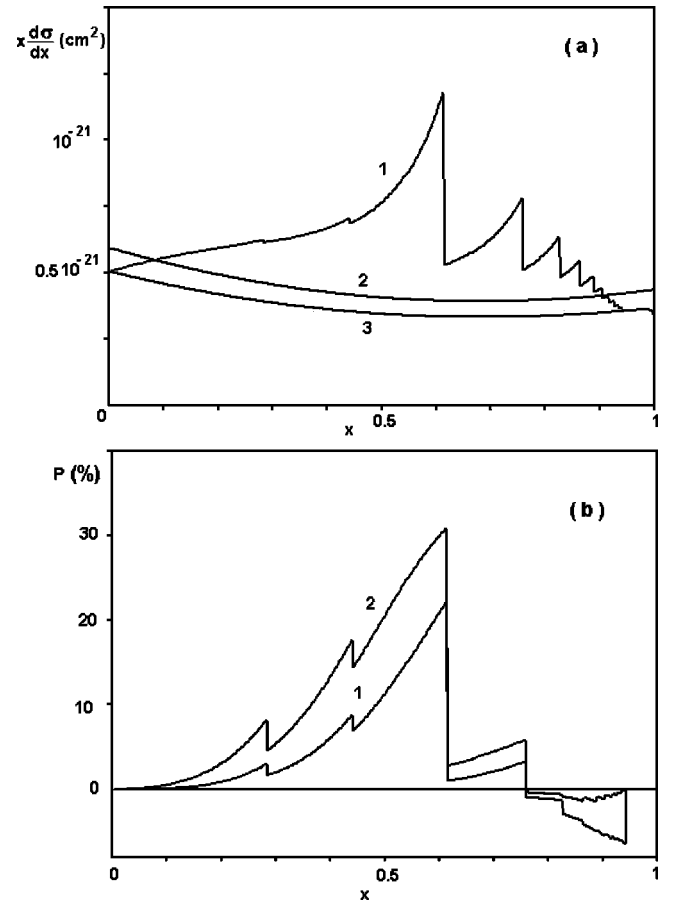


FIG. 7. (a) Differential photon spectra in a  $\text{PbWO}_4$  single crystal (1), in equivalent amorphous medium (2) and incoherent contribution (3) in the intensity as functions of the relative photon energy. (b) Degree of the linear polarization (1) and its maximum value (2). The electron energy is equal to 10 GeV. The electron beam moves in the  $(yz)$  plane (see Fig. 6) under 0.005 rad with respect to the  $z$  axis.

literature. It should be noted that this remark does not indicate a violation of the coherent mechanism. The reason is that very small deviations of the direction of the electron motion from the  $yz$  plane (at the orientations pointed out above) give a sizable contribution in the radiation intensity (at low  $x$ ).

The intensity spectra are presented for one electron energy. It is easy to understand their behavior at different energies: the incoherent contribution is practically independent of the electron energy; the coherent intensity is proportional to this energy, at the condition that the orientation angle is changed in a way inversely proportional to the energy.

The theory of coherent bremsstrahlung is violated at some orientations of atomic structures (at high enough electron energies). This problem may be investigated according to Ref. 6.

It should be noted that the calculated spectra of coherent bremsstrahlung may be interesting for applications of this effect. Despite the large volume of the fundamental cell, the radiation intensity is large enough, for rather large values of the orientation angle.

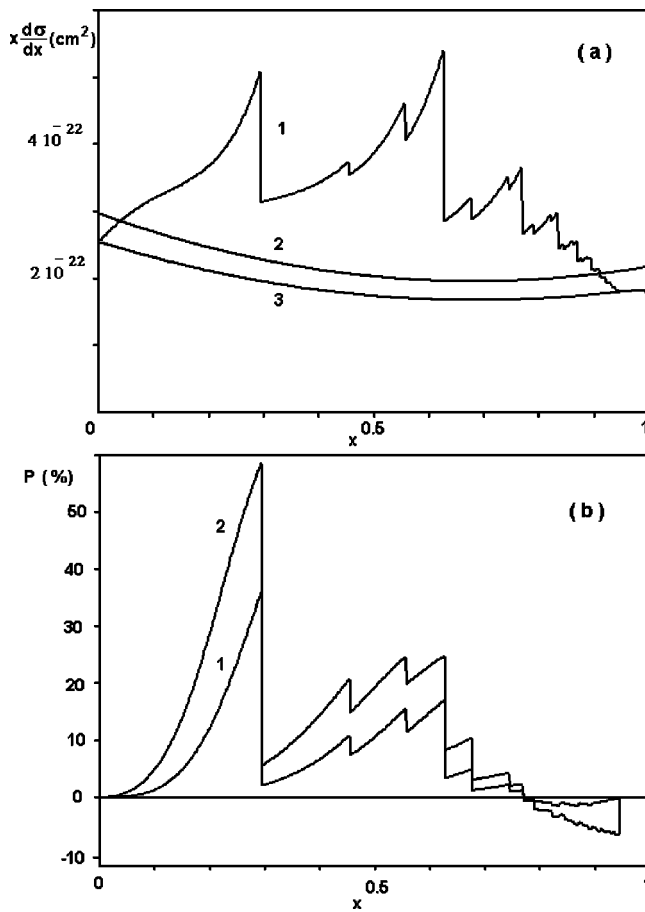


FIG. 8. The same as in Fig. 7 but for a  $\text{CaWO}_4$  single crystal.

Calculations show that the incoherent contribution in periodic atomic structures is insignificantly smaller than for the corresponding amorphous ones. However, a precise determination of the incoherent cross section may be useful, for electron energies smaller than some GeV. In this case, the emission angle of the  $\gamma$  quantum is detectable, and the in-

vestigation of the incoherent contribution may give additional information.

Our examples illustrate different types of probability density functions. For a nanotube lattice this function depends only on one coordinate, and the other coordinates are functions of the latter. The remaining examples illustrate the case when all atoms are independent.

## IX. CONCLUSION

In this paper we have shown that, in imperfect periodic atomic structures, the coherent part of the cross section is defined by the averaged potential of the structure, and the incoherent (diffusion) one is defined by the pair correlation functions. The method considered here allows one to solve the problem, on the basis of the normalized probability density function. In particular, we have calculated the cross section of coherent bremsstrahlung in polyatomic single crystals with different thermal fluctuations amplitudes. We also considered further developments of our method for atomic structures with a variable number of atoms in the cell, fluctuating periods, etc.

In this paper we did not investigate the process of coherent  $e^\pm$ -pair production in periodic structures. However, in this case there is no problem in writing similar equations as for coherent bremsstrahlung, using well known equations for the process and the relations obtained here.

On the basis of our considerations, we think that coherent bremsstrahlung and  $e^\pm$ -pair production, at particle energies between a few hundreds of MeV and some GeV, may be utilized for the investigation and characterization of the atomic structures, in parallel with other methods, such as x-ray diffraction. At these energies, the collimation of the electron beam (or the measurement of the photon angle emission) is possible, and therefore the possibility of a detailed study of pair correlations appears.

In whole, our investigations may be useful for the search of new sources of coherent radiation. The examples considered in the paper are illustrative of such a possibility.

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