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Abstract

The possibility of detection and diagnostics of nano-object parameters by means of the X-ray radiation generated at interaction of relativistic electrons with the researched object is discussed. It is shown that observation of coherent allows to research micro-structural features of electrons and nuclei distribution in nano-object. The basic conclusions are illustrated on the example of the coherent radiation by relativistic electrons on a fullerene.

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КОГЕРЕНТНАЯ РЕНТГЕНОВСКАЯ ДИАГНОСТИКА НАНО-СТРУКТУР НА ЭЛЕКТРОННЫХ УСКОРИТЕЛЯХ

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Аннотация

Обсуждается возможность обнаружения и диагностики параметров нано-объектов в веществе с помощью рентгеновского излучения, генерируемого при взаимодействии релятивистских электронов непосредственно с исследуемым объектом. Показывается, что наблюдение когерентного ПТИ и ТИ позволяет исследовать микро-структурные структурные особенности распределения электронов и ядер в нано-объекте. Основные выводы иллюстрируются на примере когерентного излучения релятивистских электронов на фуллерене.

Introduction

The main moment of nano-technology application is the reliable diagnostics of nano-structure parameters. One of the perspective methods of such diagnostics is using of X-ray radiation. This approach is based on observation (at irradiation of researched object a flux of photons) of the resonant response in intensity of dispersed photon if its wave length occurs comparable to the linear sizes of the micro-object. Technique used traditionally here, in essence, represents a version of the X-ray-structural analysis which is usually carried out by the application of a photon flux of a bremsstrahlung radiation generated by accelerated electrons on the special target-radiator.

One of the directions of the further development of radiating diagnostics is discussed below, specifically - using of the "electron - radiation" mechanism directly in researched substance. In this approach, structural properties of substance, which acts simultaneously as a bremsstrahlung radiator and the researched object , are unequivocally reveal in radiation characteristics. In such scheme, radiating diagnostics expands its possibility appreciably.

In general, arising of bremsstrahlung radiation by accelerated electrons is caused by traditional bremsstrahlung radiation (BR) on atom nuclei and polarization bremsstrahlung radiation (PB) on atom electrons of a target [1-2]. Thus in both processes the coherent phenomena, directly connected with structural features of the target substance, can be observed.

Once the wave length of a photon irradiated by a fast electron becomes comparable or surpasses characteristic atomic distances in target substance (that is observed in X-ray range), process of radiation covers several bremsstrahlung centers. This stimulates coherent generation of additional photons, phased among themselves. In the result, a coherent burst in radiation will be observed, and the wave lengths in the burst will depend sharply on the distribution of substance local concentration.

All mentioned above makes the basis for the structural diagnostics of nano-objects.

Let's note, first of all, that a total yield of generated photons and relative contributions BR and PB depend on an of radiation. So BR prevails for small angles while PB remains appreciable for the big angles including a back hemisphere [2]. Hence the observation of radiation under various angles can give the information of structure distributions of both nuclei and electrons in substance.

It is necessary also to note that specific technique allows to receive an additional information of parameters of cross and longitudinal substance distributions if it is possible to use an accelerator with a varied energy of electrons. The last circumstance is caused by distinction in dependence of cross and longitudinal characteristics of bremsstrahlung radiation on the energy of fast electrons. The matter is that process of photon radiation by an fast electron occurs on some length of electron pass in space named as coherent length of radiation L_{coh}) on which generated photon and generating electron are spatially separated. All bremsstrahlung centers "covered" by this length produce the coherent contribution to radiation with the given wave length of radiation (see, for example, [3,4], and below). The coherent length is maximal at radiation along electron velocity reaching the value $L_{coh} = 2\lambda\gamma^2$ for a photon with the wave length of λ where γ is the relativistic factor for radiating electron (strong dependence on the energy of the generating electron is observed also at all small angles of radiation). At the same time the effective cross radius of the fast electron interaction with substance grows proportionally to relativistic factor γ (see also further).

Let's specify one more important feature of the considered method. For experiments with the direct mechanism "electronic bunch - radiation" , using of intensive beams of accelerated electrons is not required. On the contrary, the application of rather weak accelerated current (up to tens - hundreds nA) is expedient due to it is quite enough for obtaining of a necessary statistical material. Simultaneously, the radiating background is reduced. So this regime allows to facilitate essentially conditions for diagnostics. Application of accelerators with high duty-factor [5] is especially perspective for this purpose.

It is necessary to mention that the features of relativistic particle radiation in substance are actively investigated in various science centers. Nevertheless, direct researches of nano-objects (molecular ions, fullerenes, nanotubes etc.) start just now (mention, for example, works of authors [6-8]).

Analytical PB description

Confirm all mentioned above by analytical estimations on an example with detection of such nano-object . At estimations, we shall be limited to basic analytical relations explaining the most typical details of considered processes. First of all, consider X-ray radiation by a relativistic electron on atomic electrons of substances, i.e. the polarization radiation process(PB) . Following to traditional procedure in which PB is represented as dispersion of own electromagnetic field of fast charge on substance electrons [9-11], we receive the following ratio for a spectrum-angular density of the radiation energy:

$$\frac{d^2 W_\omega}{d\,\omega\, d\,\Omega} \;=\; \frac{e^6}{8\,\pi^3\, m^2\, c^3\, v^2}\, F_{eff}\,, \tag{1}$$

where W_ω is the spectrum density of radiation with a frequency ω in an element $d\,\Omega$ of the solid angle. Factor

$$F_{eff} \;=\; \frac{v^2}{e^2} < |\sum_{s=1}^{Z_o} \left[\vec{n'}\,\vec{E_\omega}(\vec{r_s})\right]\, exp(-i\,\vec{q_\omega}\,\vec{r_s})\,|^2 >\,, \tag{2}$$

where Z_o is the electron number in the object, and this fact determines the total contribution of all electrons. Spatial position of each substance electron is determined by its radius $\vec{r_s}$. A vector $\vec{E_\omega}$ is the field spectral amplitude of a fast electron with the velocity $\vec{v}$.

Here the field of a fast electron is represented as a package of virtual photons [11]. Spectral amplitude of a virtual wave with the frequency ω and the wave vector $\vec{k} = \vec{v}\omega/v^2$ on a distance b from the electron trajectory has quantity [1]

$$E_\omega \;=\; \frac{e}{\pi\, b\, v}\,\zeta\, K_1(\zeta)\,,$$

where $\zeta = \frac{\omega\, b}{\gamma\, v}$, K_1 is Macdonald's function of first order. Practically, quantity of $\zeta\, K_1(\zeta) \sim 1$ at $\zeta \leq 1$, and it is decreasing sharply then at $\zeta \geq 1$. Therefore relation

$$\frac{\omega\, b}{\gamma\, v} \simeq 1 \tag{3}$$

determines, in many aspects, parameters of considered PB process . [2] So, radius of cross action of the relativistic electron field appears as

$$R_\omega \;\simeq\; \frac{\gamma\, v}{\omega} \tag{4}$$

Simultaneously, relation (4) allows to specify also limiting frequency of radiation at the given size of interaction space.

[1]Here only a cross component is taken into account; it is axial symmetric with respect to fast electron trajectory; quantity of field longitudinal component is much less.

[2]In general, the procedure described corresponds to a movement of a charge in vacuum. In a dense target, a field charge experiences influences of substance screening. We shall be limited to consideration of low relativistic electrons when the relativistic factor of particles γ and the range of radiation frequencies ω satisfy the condition $\omega^2 > \gamma^2\omega_o^2$ (here ω_o is a plasma frequency of target substance; $\hbar\,\omega_o \simeq$ 30-40 eV), and screening action is decreases.

Further, a vector $\vec{q} = \vec{k'} - \vec{k}$ where ω and $\vec{k'}$ are frequency and wave vector of a real photon (so $k' = \omega/c$) emitted in a direction of the unit vector $\vec{n'}$. At last, brackets <> mean averaging on probable positions of all electrons in a nano-object.

Factor (2) includes coherent (proportional to Z_o^2) and incoherent (proportional to Z_o) contributions of substance electrons in the total radiation. They are described the actions of pair and unpaired components in sum (2), accordingly. As actually, in any nano-object $Z_o \gg 1$, further the incoherent contribution is neglected.

In the result,

$$F_{eff} = \Big(\int\limits_{(\infty)} \frac{x\, sin(q_x\, x)\, cos(q_z\, z)}{x^2 + y^2}\, \zeta\, K_1(\zeta)\, \rho\,(\vec{r}) d\vec{r} \Big)^2 cos^2\psi, \qquad (5)$$

where $\rho\,(\vec{r})$ is an electron density of the object.

Here the Cartesian coordinates are used: $\vec{r} = (x,\, y,\, z)$, and $d\vec{r} = dx\, dy\, dz$. The z axis is directed along velocity v and passes through the object center; the unit vector of radiation $\vec{n'}$ lays in the plane (x, z) under an angle ψ with respect to the z axis. Then $q_x = \omega\, sin\Psi/c$; $q_y = 0$ $q_z = -\omega\,(1/\beta - cos\Psi)/c$ where $\beta = v/c$.

As it follows from ratios (4) and (5), there are optimum conditions at which the object electrons can give the maximal coherent contribution to total PB output. So the longitudinal and cross sizes of object and the frequency of radiation should correspond to a requirement that waves, dispersed by separate electrons, do not extinguish each other. In coherent radiation, only target electrons participate which are really "covered" by the field of fast electron. Therefore it is possible to specify two characteristic coherent lengths within the limits of which substance electrons give the synphase contribution in PB. They are so-called longitudinal coherent length $L_{\|} \sim \pi/|q_3|$ (mentioned above) and cross coherent length $L_{\perp} \sim \pi/q_1$. The effect will be maximal if the quantity of $L_{\perp}$ and the cross sizes of object at given frequency of radiation correspond to condition (4).

Analytical BR description

The same method of virtual photons can be used for a description of traditional bremsstrahlung radiation (BR) and a comparative analysis. [3] Following [9], it is possible to examine BR by a fast charge on a nucleus as

[3]Note with reference to BR that this method has rather big "experience" [12].

dispersion (in own coordinate system Σ' of a charge where the latter has no forward velocity, and the nucleus has velocity $-\vec{v}$) of an electromagnetic field of nucleus. Thus BR can be described in the system Σ' by means of "inversion" of PB formulas.

However in the situation considered, it is necessary to take into account the dispersion of a total field of all charges in a nano-object, including, besides nucleus, its electrons. Due to mutual screening of object charges, a strong suppression of BR intensity should be observed in the low-frequency range of radiation (see also [9]). Only for frequencies, when length of a wave of radiation becomes less than average distance between particles in nano-object, BR appearance is possible (but there it is weakly coherent already).

In a result, coming back to laboratory coordinate system Σ, here it is possible to note two important facts: screening of a nucleus field and narrowing of BR radiation cone. This narrowing is described by the formula

$$sin\psi \;=\; \frac{sin\psi'}{\gamma\,(1\,+\,v\,cos\psi'/c)}$$

where ψ and ψ' are radiation angles in Σ and Σ' systems, accordingly. For BR generated by relativistic electrons, all area of radiation in Σ' in a forward hemisphere is narrowed in laboratory system in a cone with the angle of $\psi\;\sim\;1/\gamma$. Thus we shall notice that the coherent BR intensity is minimal under this angle (see ratio (6)).

Nevertheless, possibility of reception of different information on nano-object structure at X-ray radiation measurements for small and big angles proves to be true.

Results and Discussion

Let's illustrate said above with concrete numerical estimations of polarization radiation (PB) by relativistic electron on such interesting nano-object as single-layered fullerene. In this case, a number of additional interference effects appear in PB. As is known, fullerene is a multiatom molecule consisting of tens - hundreds atoms of one or several sorts which are located in single or several thin layers [13]. There are fullerenes of cubic form and the most widespread spherical one. The size of single-layer fullerene is about one nm (so the most widespread fullerene C_{60} has diameter 0.7 nm).

Results of numerical modelling of PB by relativistic electron on cubic single-layer fullerene with an edge $d\;=\;0.7$ nm are submitted in Fig. 1. As all atoms of this object are located on its surface, PB is a result of interference additions of radiation signals from all object surfaces. Here is traced following characteristic trend in dependence of the factor F_{eff} (the latter here and in the subsequent figures is presented in relative units per one electron of nano-object) on energy of emitted photons.

In low-frequency area where length of a radiation wave λ is more than sizes of object (i.e. at energy of photon $E_\omega \lesssim 2$ keV), all fullerene electrons are radiating practically in unison that results in appearance of sharp PB peak.

At bigger photon energies, radiating surfaces of fullerene appear in mutually extinguishing phases that results in PB suppression (at $q_3\, d \sim \pi$, see curve (3) in Fig. 1). Further " game of phases " results in occurrence several oscillations of PB intensity with gradual attenuation of their amplitudes (double influence of coherence reduction and high-frequency attenuations of a relativistic electron field, see. (4); third maximum - result of full concurrence of radiation phases from the front and back walls of object).

Similar dependences for spherical fullerene C_{60} with diameter $d = 0.7$ nm are submitted in Fig. 2 for two cases: usual thin-layer fullerene (curve 1) and one with internal infilling (curve 4). As average distance between front and back hemispheres is here less d, a width of the basic coherent peak (curve 1) is more than one at cubic fullerene. This fact has even more effect in the second case where the width of coherent peak reaches up to 3 keV. Besides, there is one more circumstance in the last case - more close position (on the average) of fullerene electrons to a trajectory of incident electron. Hence its field has stronger influence that is reflected in higher amplitude of a signal in curve 4.

Dependence of factor F_{eff} for single-layer fullerene C_{60} on photon energy for various relativistic factors of incident electron for angles $\psi = \pi/4$ (curves 1,2,3) and $\psi = \pi\, 3/4$ (curve 4) is indicated in Fig. 3.

One can note a saturation of coherent peak amplitude (i.e. of factor F_{eff}) that quite corresponds to discussed representations about character of radiation by relativistic electron. Really, here the longitudinal coherent length of radiation $L_{\mid}$ becomes comparable at photon energy about one keV with fullerene diameter already for the relativistic factor about ten.

The increase of peak connected to growth $L_{\mid}$ at the big values relativistic factor can take place only in more complex systems, for example, in a fullerene chain when the coherent length gradually "covers" the next objects.

Confirmation of said follows also from comparison of curves 2 and 4. At radiation under angle $\psi = \pi\, 3/4$ the q_3 appreciably grows, and $L_{\mid}$ decreases. Therefore the amplitude of a coherent signal sharply fades, and the oscillation period of its amplitude decreases.

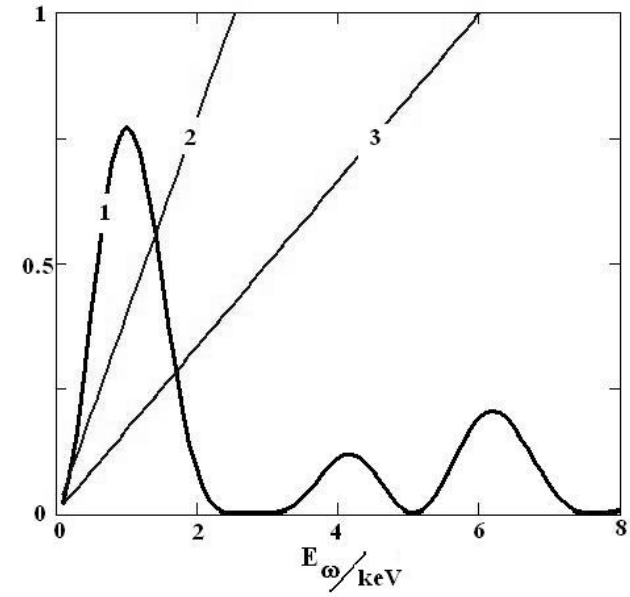

Figure 1: Dependence of PB parameters by fast electron with the relativistic factor $\gamma = 10$ on photon energy for cubic single-layer fullerene with the edge $d = 0.7$ nm at the radiation angle $\psi = \pi/4$: curve 1 - the factor F_{eff} (arb. un.); curves 2,3 - the cross and longitudinal reduced phases $q_1\, d/2\pi$ and $q_3\, d/2\pi$, accordingly.

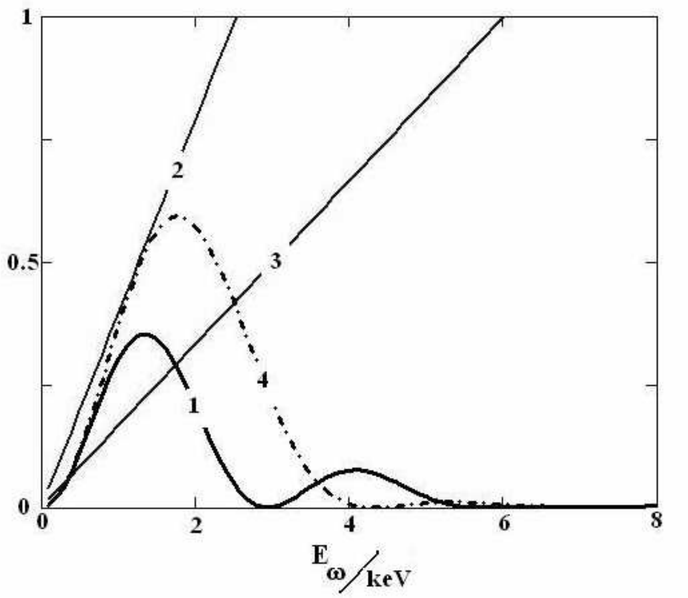

Figure 2: Dependence of PB parameters by fast electron with the relativistic factor $\gamma = 10$ on photon energy for spherical fullerene with diameter $d = 0.7$ nm for different distributions of its atoms at the radiation angle $\psi = \pi/4$): curves 1,4 - factors F_{eff} (arb. un.) for single-layer fullerene and one with internal infilling by atoms; curves 2,3 - the cross and longitudinal reduced phases $q_1\, d/2\pi$ and $q_3\, d/2\pi$, accordingly.

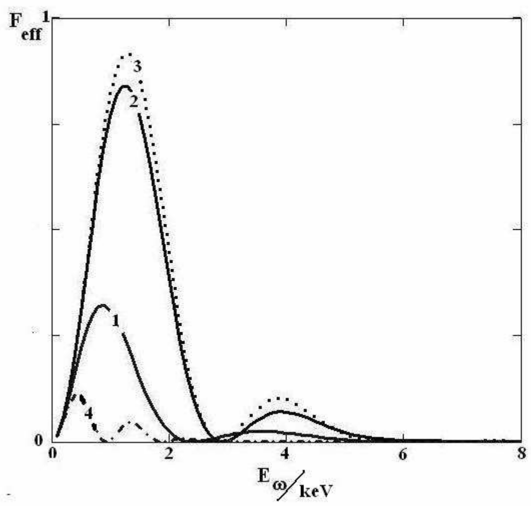

Figure 3: Dependence of factor F_{eff} (arb. un.) in PB by fast electron with different relativistic factors γ on photon energy for spherical single-layer fullerene C_{60} with diameter $d = 0.7$: curves 1,2,3 - the radiation angle $\psi = \pi/4$ and $\gamma = 10, 50, 100$, accordingly; curve 4 - the radiation angle $\psi = 3\pi/4$ and $\gamma = 10$.

Thus the numerical estimations confirm qualitative assumptions about possibilities of coherent radiating diagnostics of nano-objects. Let's remind that amplitude of coherent radiation by relativistic electrons on nano-objects is proportional to a square of its number electrons. So, for example, intensity PB on fullerene C_{60}in $(60)^2$ times exceeds a level of similar signal on single atom of carbon (!).

Nevertheless questions of more detailed studying of the substance containing nano-objects, the analysis of more complex nano-complexes and so on demand the further researches.

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