

**Transition radiation from electrons: Application to thin film and superlattice analysis**I. D. Feranchuk<sup>1,\*</sup> and A. Ulyanenko<sup>2,†</sup><sup>1</sup>*Byelorussian State University, Franciska Skariny Avenue 4, 220050 Minsk, Republic of Belarus*<sup>2</sup>*Bruker-AXS, Östliche Rheinbrückenstrasse 50, 76187 Karlsruhe, Germany*

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The transition radiation from nonrelativistic electrons moving in periodical nanostructures is discussed in view of its application to surface and interface analysis and thickness measurements. The spectrum of this radiation is shown to deliver information on the investigated sample that is similar to that provided by conventional x-ray reflectivity methods. An analytical expression for the intensity of electromagnetic radiation from the electrons passing through the periodical multilayers has been derived. Numerical examples of radiation spectra are given for some typical sample models, and general conditions for the observation of these spectra with a background of bremsstrahlung are discussed.

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**I. INTRODUCTION**

Ultrarelativistic electrons ( $E > 50$  MeV) interacting with periodic media yield the radiation spectrum, which is almost equivalent to the resulting pattern of the coherent quasimonochromatic x-ray beam scattered by the same media.<sup>1,2</sup> The spectrum of x-ray radiation from medium-energy electrons with  $E = 0.1 - 10$  MeV, moving within the crystal, has been recently shown<sup>3-5</sup> to be determined by the same structure amplitudes, which define the intensity of the diffracted x-ray beam in the crystal.

In accordance with the results of Refs. 3 and 4, the principal advantage of radiation, produced by the electron beam immediately inside the investigated crystal, is the reduction of detection time in comparison with recording time for conventional diffraction curves obtained with laboratory x-ray sources. The physical reason for such an intensity gain is the transference of the point, where the energy of the electrons transforms to the radiation. In the proposed method, the x rays are produced when the electron's electromagnetic field is scattered by the atoms of the investigated media. In conventional experiments with x-ray tubes, this conversion takes place in the anode of the tube (with the effectiveness essentially less than unity), and then x rays are transported to the sample to be scattered. Recent publications<sup>6-8</sup> confirm the interest of the scientific community in the application of radiation from relativistic electrons to a characterization of nanostructures.

In the present paper, we discuss the possibility of an application of the transition radiation (TR) from nonrelativistic electrons to investigation of superlattices and thin solid films, which is usually carried out by a conventional x-ray reflectometry method. The generation of photons in the TR mode is determined by an abrupt change of permittivity when a moving electron crosses the border between different media. This phenomenon has been studied theoretically<sup>9,1</sup> in the general case and experimentally for the optical range of wavelengths,<sup>1</sup> where the kinematical features of TR are similar to the features of inverse photoemission. However, the physical principles of the formation of both radiations are essentially different. Whereas the inverse photoemission is determined by the radiative transitions of moving electrons

onto vacant energy levels within the media,<sup>10,11</sup> the transition radiation is produced even in the case of constantly moving charged particles, and the intensity of TR depends on the polarization of the whole media. In the x-ray range, the permittivity of the media depends universally on the radiation frequency and is proportional to the electron density.<sup>12</sup> This fact makes it possible to use the TR spectrum for determination of the principal parameters of the nanoscale multilayered structures. We demonstrate that the amplitudes of the wavefields of TR photons are determined by expressions similar to those in the case of x-ray scattering on the same sample. However, contrary to the scattering problem, the TR spectrum is observed with a background of bremsstrahlung (BS), which is caused by multiple scattering of electrons within the media. Therefore, we also derive the universal formula connecting the intensity of both radiations (see also Ref. 4). This allows us to determine the range of wavelengths in which the TR spectrum becomes visible on the BS background and to identify this range as 5–50 nm, i.e., comparable with the typical size of the imperfections (interface roughness, stepped interfaces, etc.) and inhomogeneity (layered structure of the sample) within the nanostructures. The essential point is found to be an observation angle of TR, viz., the angle between the sample surface and the detector. The value of this angle must be small enough to register the TR photons emitted from the only short part of the electron's trajectory, which diminishes the BS and multiple scattering, as has been proved for optical TR.<sup>1</sup> In Sec. III, we derive an analytical expression for the spectral intensity of TR from an electron beam passing through the periodic multilayered structure and we give a numerical example of simulated TR spectra for typical nanostructures. The examples demonstrate the difference of the proposed technique from traditional methods, e.g., x-ray reflectivity measurements. In the latter case, the information on the depth profile of nanostructure (layer thicknesses) is determined from the position of the peaks in an angular distribution of reflected x-ray intensity, which requires the usage of a goniometer in the experiment. In the proposed technique, the analogous information is contained in the frequency dependence of radiation, which can be recorded at a fixed position of the detector. Besides the thickness profile, TR intensity depends also on the imperfec-

tions of the interfaces (for example, roughness) within the nanostructure.

## II. INTENSITY OF TRANSITION RADIATION FROM ELECTRON IN NANOSTRUCTURE

In the general case, the exact solution for the problem of TR from a charged particle moving within the stack of plates<sup>13</sup> can be used for the derivation of wavefield amplitudes. However, the expression for this solution is cumbersome, which complicates the qualitative physical analysis. Therefore, we derive the formula for radiation intensity in a more reductive form to establish the relationship between the radiation from electrons in the multilayers and scattering of x rays from the same structure. We also restrict our consideration to the samples, the permittivity of which is close to unity.

The intensity of radiation follows from the general formula for the cross section of electromagnetic processes in arbitrary media.<sup>2</sup> Neglecting the scattering of electrons inside the sample and the influence of refraction on the polarization of radiation, the expression for the spectral density of the photon number with frequency  $\omega$  emitted in the direction  $\mathbf{n}$  in a unit time can be written as<sup>2</sup>

$$\frac{\partial^2 N}{\partial \omega \partial \mathbf{n}} = \frac{e^2 \omega}{4 \pi^2 c^2} J \left[ 1 - \left( \frac{\mathbf{nv}}{c} \right)^2 \right] \times \left| \int_{-\infty}^{+\infty} dz \exp[i(p_z - p_{1z})z/\hbar] U_{\mathbf{k}}^{(-)*}(z) \right|^2. \quad (1)$$

Here  $\hbar$  is the Planck constant,  $c$  is the velocity of light,  $\mathbf{k} = \omega/c\mathbf{n}$ ,  $J$  is the number of electrons with energy  $E$ , and velocity  $\mathbf{v} = c^2\mathbf{p}/E$ , striking the sample at angle  $\beta$  in unit time;

$$p_z = \sqrt{E^2/c^2 - m^2 c^2 - p_x^2 - p_y^2},$$

$$p_{1z} = \sqrt{(E - \hbar \omega)^2/c^2 - m^2 c^2 - (p_x - \hbar k_x)^2 - (p_y - \hbar k_y)^2}$$

are the projections of the primary and final momentum of the electron to the  $z$  axis, which is an outward normal to the sample surface (Fig. 1).

The scalar function  $U_{\mathbf{k}}^{(-)}(z)$  describes the amplitude of the electromagnetic field, corresponding to the solution of the uniform Maxwell equations for the wave falling from vacuum on the sample at angle  $\alpha$ . A formation of the radiation amplitude by an inverse wave follows from the general theory of the  $S$  matrix,<sup>2</sup> the particular case of which is the reciprocity theorem used for a description of diffuse x-ray scattering.<sup>14</sup> The wave  $U_{\mathbf{k}}^{(-)}(z)$  can be represented as a combination of transmitted and specularly reflected waves with amplitudes, determined by recurrent equations,<sup>15</sup> widely used in x-ray reflectometry. This wave is certainly the unique solution of Maxwell's equations for a monochromatic wavefield. However, the form of this solution is inconvenient for calculation of the radiation intensity for different frequencies because for every photon's wave vector, the recurrent procedure must be applied. Meanwhile, there is an exact analytical

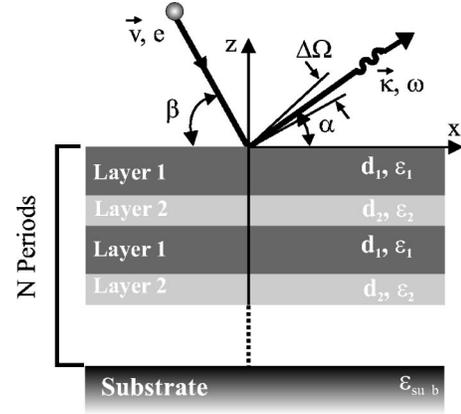


FIG. 1. Schematic view of the general sample model and beam directions. An electron beam of velocity  $\mathbf{v}$  and charge  $e$  falls on the sample at angle  $\beta$ , and the photons  $(\mathbf{k}, \omega)$  are detected at exit angle  $\alpha$  by a detector with aperture  $\Delta\Omega$ .

representation for the wavefield, which can be effectively applied for the present problem, and we revisit it in brief below.

Let us consider first the stationary states of an electromagnetic wave inside the infinite periodical media consisting of a stack of bilayers with permittivities of upper and lower parts to be denoted by  $\epsilon_1$  and  $\epsilon_2$ , respectively. The wave of frequency  $\omega$  propagates with angle  $\alpha$  to the sample surface. The solution for this problem is analogous to the Kronig-Penney problem in quantum mechanics. Inside the single bilayer period of number  $l$ , it can be represented using transmission  $T_l$  and reflection  $R_l$  coefficients<sup>15</sup> and Bloch functions:

$$\psi(z) = e^{i\kappa z} u(z), \quad u(z+d) = u(z), \quad d = d_1 + d_2, \quad (2)$$

where the periodical function  $u(z)$  is

$$u(z) = a e^{i\chi_1 z} + b e^{-i\chi_1 z} = [T_l e^{i\chi_1 z} + R_l e^{-i\chi_1 z}] e^{-i\kappa z}, \quad 0 < z < d_1, \\ u(z) = a' e^{i\chi_2 z} + b' e^{-i\chi_2 z} = [T_l' e^{i\chi_2 z} + R_l' e^{-i\chi_2 z}] e^{-i\kappa z}, \quad d_1 < z < d, \quad (3)$$

$$\chi_{1,2} = k \sqrt{\epsilon_{1,2} - \cos^2 \alpha}, \quad k = \frac{\omega}{c}.$$

It is important that none of the coefficients  $a, b, a', b'$  depends on the layer position within the stack. Their values are defined by known analytical expressions, following from the conditions of the periodicity for  $u(z)$ , its derivative, and the continuity of the wavefield at the interfaces between the layers. Bloch parameters  $\kappa_{1,2}$  are the solutions to the dispersion equation:

$$\cos \kappa d = \cos \chi_1 d_1 \cos \chi_2 d_2 + \frac{\chi_1^2 + \chi_2^2}{2\chi_1 \chi_2} \sin \chi_1 d_1 \sin \chi_2 d_2. \quad (4)$$

For every frequency  $\omega$  and angle  $\alpha$ , this transcendental equation defines two independent linear waves  $\psi_{1,2}(z)$ , corresponding to the values  $\kappa_{1,2} = \pm \kappa$ . The coefficients in Eq. (3), being normalized by condition  $a = 1$ , are determined from the following formulas:

$$\begin{aligned} T_l &= e^{-i\chi_1 l d}, \quad R_l = b e^{i\chi_1 l d}, \quad T'_l = a' e^{-i\chi_2(l+1)d}, \\ R'_l &= b' e^{i\chi_2(l+1)d}, \\ b &= \frac{(\chi_1 + \chi_2)[e^{i\kappa d} - e^{i(\chi_1 d_1 + \chi_2 d_2)}]}{(\chi_1 - \chi_2)[e^{i\kappa d} - e^{i(-\chi_1 d_1 + \chi_2 d_2)}]}, \\ a' &= \frac{\chi_2 + \chi_1 + (\chi_2 - \chi_1)b}{2\chi_2} e^{i\kappa d}, \\ b' &= \frac{\chi_2 - \chi_1 + (\chi_2 + \chi_1)b}{2\chi_2} e^{i\kappa d}. \end{aligned} \quad (5)$$

In the range of x-ray wavelengths, where the condition  $|\epsilon - 1| \ll 1$  is fulfilled, the expression for parameters  $\kappa_{1,2}$ , defining two linearly independent solutions for Maxwell's equations for periodical media, can be found in obvious analytical form:<sup>16</sup>

$$\kappa_{1,2} d = \pi n + \delta_{1,2}, \quad \chi_1 d_1 + \chi_2 d_2 = \pi n + \nu, \quad (6)$$

$$\delta_{1,2} = \pm \sqrt{\nu^2 - \frac{|\chi_1 - \chi_2|^2}{2|\chi_1 \chi_2|} |\sin \chi_1 d_1|^2}. \quad (7)$$

These approximate solutions are equivalent to the two-wave approximation of dynamical diffraction theory for one-dimensional periodical media and are valid only for grazing angles of the photon velocity vector to the plane of layers, exceeding the critical angle of total external reflection (TER)  $\theta_{cr}$  for every plate (layer), i.e., when the conditions are fulfilled,

$$\alpha > \sqrt{|\epsilon_i - 1|}, \quad \chi_i d_i \sim 1, \quad i = 1, 2.$$

These conditions are shown below to be the principal ones for the radiation problem. When they are satisfied, the reflection coefficient from every layer is small enough and the wave transmission is determined by Bragg reflections, which

are caused by normal periodicity of the sample. If either the incident angle  $\beta$  or the exit angle  $\alpha$  is close to the critical angle of TER, the general equation (4) must be used instead of Eq. (6).

The function  $U_{\mathbf{k}}^{(-)}(z)$  describing both the scattering of the wave from the stack of plates and the cross section of x-ray radiation from electrons inside the stack can be found from stationary states of an electromagnetic field in the sample by using the boundary conditions at the sample surface and at the top interface of the substrate:

$$\begin{aligned} U_{\mathbf{k}}^{(+)}(z) &= U_{-\mathbf{k}}^{(-)*}(z) = e^{ik \sin \alpha z} + R_0 e^{-ik \sin \alpha z}, \quad z > 0, \\ &= T\psi_1(z) + R\psi_2(z), \quad -Nd < z < 0, \\ &= T_f e^{i\chi_f z}, \quad \chi_f = k\sqrt{\epsilon_f - \cos^2 \alpha}, \quad z < -Nd. \end{aligned} \quad (8)$$

The approach presented above permits us to find the wavefield at every point of the sample without solving the system of recurrent or matrix equations. This also may be useful for the calculation of the diffuse scattering cross section by the distorted-wave approximation.<sup>14</sup> Finally, for calculation of the reflection  $R_0, R$  and transmission  $T, T_f$  integral coefficients for all structures, the system of linear equations following from the continuity conditions is used:

$$\begin{aligned} 1 + R_0 &= T(1 + b_1) + R(1 + b_2), \\ k \sin \alpha (1 - R_0) &= T[(\kappa + \chi_1) + (\kappa - \chi_1)b_1] + R[(-\kappa + \chi_1) - (\kappa + \chi_1)b_2], \end{aligned} \quad (9)$$

$$\begin{aligned} T_f e^{i\chi_f Nd} &= T e^{i\kappa(N-1)d} (a'_1 e^{i\chi_2 d} + b'_1 e^{-i\chi_2 d}) \\ &\quad + e^{-i\kappa(N-1)d} R (a'_2 e^{i\chi_2 d} + b'_2 e^{-i\chi_2 d}), \end{aligned}$$

$$\begin{aligned} \chi_f T_f e^{i\chi_f Nd} &= T e^{i\kappa(N-1)d} [(\kappa + \chi_2)a'_1 e^{i\chi_2 d} \\ &\quad + (\kappa - \chi_2)b'_1 e^{-i\chi_2 d}] + e^{-i\kappa(N-1)d} R \\ &\quad \times [(-\kappa + \chi_2)a'_2 e^{i\chi_2 d} - (\kappa + \chi_2)b'_2 e^{-i\chi_2 d}]. \end{aligned}$$

Here the coefficients  $a_i, b_i$ ,  $i = 1, 2$  follow from formulas (5) when Bloch's parameter takes the values  $(\pm \kappa)$ . The coefficients  $R_0$  and  $T_f$  follow from Eqs. (9),

$$\begin{aligned} R_0 &= \frac{A_2^-(\kappa)B_1(\kappa) - A_1^-(\kappa)B_2(-\kappa)}{A_1^+(\kappa)B_2(-\kappa) - A_1^+(\kappa)B_1(\kappa)}, \\ T_f e^{i\chi_f d} &= e^{i(\kappa - \chi_f)(N-1)d} \frac{[\Delta_2'(\kappa)(\alpha'_1 + \beta'_1) - \Delta_1'(-\kappa)(\alpha'_2 + \beta'_2)]}{[\Delta_2(\kappa)(1 + \beta_1) - \Delta_1(-\kappa)(1 + \beta_2)]} \frac{[\Delta_2(1 + R_0) - k \sin \alpha (1 + \beta_2)(1 - R_0)]}{[(\chi_2 - \kappa)\alpha'_2 - (\chi_2 + \kappa)\beta'_2] - \chi_f(\alpha'_2 + \beta'_2)}, \\ A_{1,2}^{(\pm)}(\kappa) &= [(\chi_1 - \kappa \pm k \sin \alpha) - \beta_{1,2}(\chi_1 + \kappa \mp k \sin \alpha)] e^{i\kappa(N-1)d}, \\ B_{1,2}(\kappa) &= (\chi_2 + \kappa - \chi_f)\alpha'_{1,2} - (\chi_2 - \kappa + \chi_f)\beta'_{1,2}, \\ \Delta'_{1,2}(\kappa) &= (\chi_2 - \kappa)\alpha'_{1,2} - (\chi_2 + \kappa)\beta'_{1,2}, \quad \Delta_{1,2}(\kappa) = (\chi_1 - \kappa) - (\chi_1 + \kappa)\beta_{1,2}. \end{aligned} \quad (10)$$

### III. QUALITATIVE ANALYSIS OF THE SPECTRAL INTENSITY OF RADIATION

In conventional reflectometry, the quasimonochromatic characteristic radiation is used and the angular dependence of scattered photons is studied. In the proposed ‘‘radiation’’ approach, the energy spectrum of x rays is wide enough, which makes the experiments with a fixed position of a detector, which records the spectral distribution of radiation more advantageous. In this scheme, the spectral density of emitted photons can be found after the substitution of a wavefield from Eq. (9) into Eq. (1) and further integration over the solid angle  $\Delta\Omega$ , determined by the width of the detector slit (for simplicity, the normal incidence of electrons is considered here,  $\beta = \pi/2$ ):

$$\frac{dN}{d\omega} = \frac{e^2 v^2 \cos^2 \alpha \sin^2 \alpha}{4\pi^2 c^2 \omega} J\Delta\Omega |M(\omega, \alpha)|^2,$$

$$M = \frac{1}{1 + \frac{v}{c} \sin \alpha} + \frac{R_0}{1 - \frac{v}{c} \sin \alpha} - \frac{T_f}{1 + \frac{v\chi_f}{kc}} e^{i[k + (v/c)\chi_f]Nd}$$

$$- \left[ \frac{1 - \exp i\left(k + \frac{v}{c}\kappa\right)Nd}{1 - \exp i\left(k + \frac{v}{c}\kappa\right)d} TL_1 \right. \\ \left. + \frac{1 - \exp i\left(k - \frac{v}{c}\kappa\right)Nd}{1 - \exp i\left(k - \frac{v}{c}\kappa\right)d} RL_2 \right]. \quad (11)$$

The parameters  $L_{1,2}$  in Eq. (11) define the amplitude of radiation from electrons passing a single period of the nanostructure and are expressed analytically through the coefficients  $a_s$ ,  $a'_s$ ,  $b_s$ , and  $b'_s$  ( $s=1,2$ ):

$$L_s = a_s \frac{e^{i[k \pm (v/c)\kappa + (v/c)\chi_1]d_1 - 1}}{1 \pm \frac{v}{kc} \kappa + \frac{v}{kc} \chi_1}$$

$$+ b_s \frac{e^{i[k \pm (v/c)\kappa - (v/c)\chi_1]d_1 - 1}}{1 \pm \frac{v}{kc} \kappa - \frac{v}{kc} \chi_1}$$

$$+ a'_s \frac{e^{i[k \pm (v/c)\kappa + (v/c)\chi_2]d_2 - 1}}{1 \pm \frac{v}{kc} \kappa + \frac{v}{kc} \chi_2}$$

$$+ b'_s \frac{e^{i[k \pm (v/c)\kappa - (v/c)\chi_2]d_2 - 1}}{1 \pm \frac{v}{kc} \kappa - \frac{v}{kc} \chi_2}.$$

All the terms in Eqs. (11) have a certain physical interpretation. The first and the second terms describe the radiation<sup>2</sup>

resulting from the reflection of pseudophotons, composing the electromagnetic field of electrons, from the surface of the sample. The intensity of this radiation depends on the same reflection coefficient  $R_0$ , which determines the intensity of the specular beam in x-ray reflectometry. Thus, to obtain comprehensive information about the surface of the nanostructure, the radiation from electrons should be detected in the direction  $R_0 \rightarrow 1$ .

The third term describes the radiation originating in the substrate, and its amplitude tends to zero with an increasing number of layers, if the absorption is taken into account. Finally, the last two terms are responsible for radiation formed inside the multilayers. The corresponding amplitude contains sharp peaks caused by the interference of radiation from different layers, which is the so-called resonant radiation.<sup>1,13</sup>

In our paper, we consider the medium-energy electrons  $E \approx 0.1-1.0$  MeV, which makes it possible to operate with intense electron beams. Three limiting cases of the investigated structure are considered below, when Eq. (11) takes the following very simple form: (i) the multilayered structure is absent and electrons radiate the photons only when crossing the substrate surface, (ii) the number of superlattice periods  $N \gg 1$ , and (iii) a single thin plate (film) without a substrate.

In the former case, Eq. (11) is reduced to well-known formulas for transition radiation,<sup>17</sup> which are valid for the angles of emitted photons close to the value of  $\theta_{cr}$ , where the reflection coefficient  $R_0 \sim 1$ . Neglecting the imaginary part, the permittivity of the substrate can be defined as

$$\epsilon_f = 1 - \frac{\omega_0^2}{\omega^2},$$

$$\omega_0^2 = \frac{4\pi e^2 \rho}{m}, \quad (12)$$

$$\alpha \sim \alpha_c = \frac{\omega_0}{\omega} \ll 1,$$

where  $\rho$  is the electron density of the substrate material. Then the spectral density of emitted photons, in the approximation of grazing incident angles, is written as

$$F(\omega) = \omega^3 \frac{dN}{d\omega} = A \frac{\omega_0^4}{[\omega + \sqrt{\omega^2 - \omega_0^2/\alpha^2}]^2}, \quad \omega > \omega_0/\alpha,$$

$$= A \omega_0^2 \alpha^2,$$

$$\omega < \omega_0/\alpha,$$

$$A = \frac{e^2 v^2 (1 - v^2/c^2)^2}{c^2 \pi^2} J\Delta\Omega. \quad (13)$$

The real application of the proposed technique for the investigation of surfaces has some limitations because the

TR spectrum is recorded with an intensive background of incoherent bremsstrahlung caused by multiple scattering of electrons within the sample. Therefore, it is necessary to estimate for which radiation frequency and media parameters the TR spectrum is observable on this background. For this purpose, we use a known formula for the cross section of bremsstrahlung<sup>18</sup> and derive an expression for the spectral density of BS photons normalizing the values in the same way as in Eqs. (13):

$$\left(\frac{dN}{d\omega}\right)_{\text{BS}} \simeq \frac{e^2 Z^2}{\pi} \left(\frac{e^2}{mc^2}\right)^2 \ln(183Z^{-1/3}) \rho_a L_{\text{abs}} \alpha J \frac{\Delta\Omega}{\omega}. \quad (14)$$

Here  $\rho_a$  is the number of atoms with a nucleus of charge  $Z$  in the unit volume,  $\rho = Z\rho_a$ , and  $L_{\text{abs}}$  is the absorption length of media for frequency  $\omega$ . The coefficient  $L_{\text{abs}}\alpha$  determines part of the electron's trajectory, the radiation from which contributes to the recorded data. The electron is assumed to fall on the sample perpendicular to the surface, and the detector makes the angle  $\alpha$  with the sample surface. It should also be noted that a similar weakening of bremsstrahlung intensity at the grazing angles is well known from experiments on TR in the optical range.<sup>1</sup> Using Eq. (14), the ratio  $\xi$  of TR and BS spectral densities is expressed as

$$\xi \simeq \frac{16\pi v^2 c^2 (1-v^2/c^2)^2 \rho_a}{\omega^4 L_{\text{abs}}(\omega) \alpha \ln(183 \cdot Z^{-1/3})}. \quad (15)$$

Evidently, the possibility of TR observation is conditioned by the inequality  $\xi > 1$ , which establishes the upper limit for the frequency of emitted photons. Substituting the real values for Si crystal in Eq. (15),

$$Z = 14, \quad \rho_a = (5.43)^{-3} 10^{24} \text{ cm}^{-3}, \quad \alpha = 10^{-2},$$

$$L_{\text{abs}} \simeq 3 \times 10^{-5} \times (\hbar\omega, \text{keV})^3 \text{ cm},$$

and assuming the energy of electrons is  $E > 0.1$  MeV, the TR intensity is observable under the following conditions:

$$\hbar\omega < 0.5 \text{ keV}, \quad \lambda = \frac{2\pi c}{\omega} > 3 \text{ nm}. \quad (16)$$

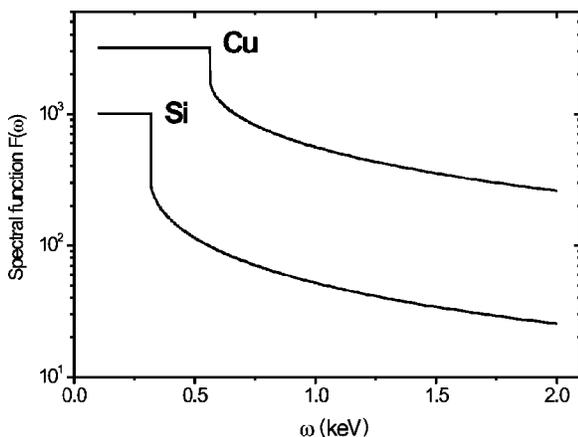


FIG. 2. Simulated spectral function of radiation from nonrelativistic electrons within the silicon and copper crystals.

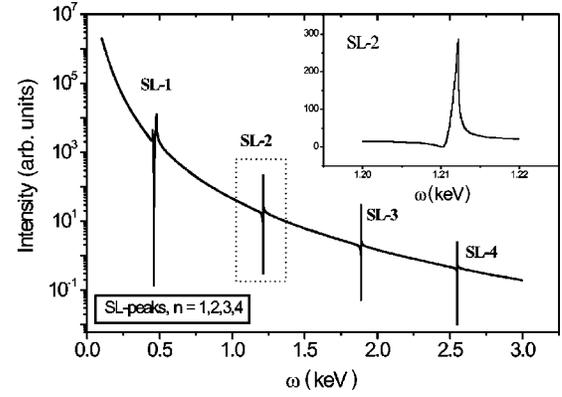


FIG. 3. Calculated intensity of x-ray radiation from electrons in the Mo/Si superlattice. The superlattice Bragg peaks are marked as SL- $n$  and the inset shows the fine structure of SL-2.

These values are typical for any material used in modern semiconductors and the estimate predicts the observation of TR in the range of soft x rays. Of course, the wavelength of radiation should be comparable with the characteristic size of the investigated inhomogeneity, e.g., stacking of materials in multilayers, vertical or lateral correlation lengths, interface stepping, etc. Thus, at some conditions, TR spectra can be used along with or instead of conventional x-ray reflectivity and diffraction methods.

Figure 2 demonstrates the radiation spectra of electrons within the silicon and copper substrates. The appearance of curves is similar to the dependence of the reflectivity coefficient on the incidence angle for x-ray scattering,<sup>12</sup> and the spectral function contains information about the surface and the density profile of the sample that is analogous to that obtained from x-ray reflectivity. The absolute spectral intensity of the photon flux reaches  $\sim 10^2$  quantum/keV sec for 100-keV electrons with current  $10 \mu\text{A}$  within solid angle  $\Delta\Omega \simeq 10^{-3}$  rad.

The second limiting case is the superlattice with a large number of periods, when the condition  $\omega_0 N d \gg 1$  is fulfilled. Assuming the photons exit angle is larger than  $\theta_{\text{cr}}$ , the radiation spectrum does not depend on  $N$  and contains peaks corresponding to the Bragg reflections from a vertical one-

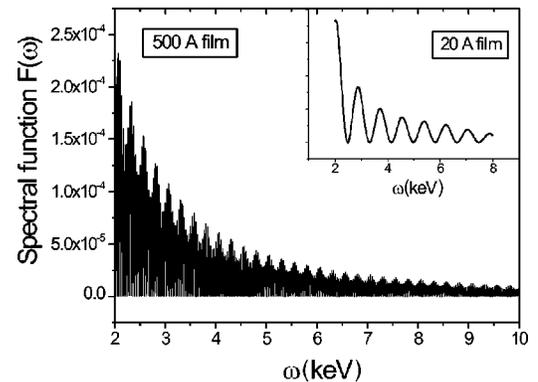


FIG. 4. Calculated spectral function of x-ray radiation from electrons, crossing the copper plate of finite thickness  $500 \text{ \AA}$  and  $20 \text{ \AA}$  (inset). Two types of oscillations are visible in both curves (for details, see the text).

dimensional periodical structure, i.e., a bilayered superlattice. The positions of the peaks are defined by the condition

$$\frac{\omega}{c}[d_1\chi_1 + d_2\chi_2] = \pi n, \quad n=0,1,2,\dots \quad (17)$$

In the vicinity of the  $n$ th superlattice Bragg peak, Eq. (11) is transformed to

$$\frac{dN_n}{d\omega} = \frac{e^2 v^2 n^2}{4\omega c^2} \left| \frac{\tilde{\epsilon}_1 d_1 + \tilde{\epsilon}_2 d_2}{(d_1 + d_2)(\nu + \delta)} \left( \frac{\tilde{\epsilon}_1 d_1 + \tilde{\epsilon}_2 d_2}{d_1 + d_2} - \frac{2\nu}{\pi n} \right) \right|^2. \quad (18)$$

Here, the parameters  $\nu$  and  $\delta$  define the deviation of radiation frequency from the Bragg condition (17) and are determined by Eq. (6);  $\epsilon_{1,2} = \epsilon_{1,2} - 1$ . The simulated radiation

spectrum from the Mo/Si superlattice is shown in Fig. 3. The Mo and Si layers are 39 Å and 58 Å thick, respectively. The detector is positioned at  $\alpha = 0.1$  rad, and electrons of energy  $E = 100$  keV and current  $J = 50$  μA fall perpendicular to the surface of the superlattice. The superlattice Bragg peaks are denoted SL- $n$ , and the inset shows the fine structure of SL-2. The integral number of photons in the  $n$ th Bragg peak is the same amount as the above-mentioned value for the radiation from electrons passing through the single surface.

Finally, the single plate is the limiting case of a thin film on a substrate, when the density of the former essentially exceeds the density of the latter. The spectral function of radiation in this case is written as

$$F(\omega) = \omega^3 \frac{dN}{d\omega} = A \omega_0^4 \frac{\omega^2 + x_0^2 - \frac{\omega_0^2}{\alpha^2} \cos^2 \mu - 2x_0^2 \cos \mu \cos \nu - 2\omega x_0 \sin \mu \sin \nu}{(x_0^4 + \omega^4) \sin^2 \mu + 4\omega^2 x_0^2}, \quad (19)$$

where  $x_0 = \sqrt{\omega^2 - \omega_0^2/\alpha^2}$ ,  $\mu = d\alpha x_0/2v$ , and  $\nu = \omega d/2v$ . Equation (19) is valid when the frequency of radiation obeys the inequality  $\omega > \omega_0/\alpha$ , which cuts off the region below the critical angle of TER for the plate. Figure 4 demonstrates the simulated spectra from 500 Å and 20 Å (inset) copper films. The electrons of 100 keV with current 50 μA strike the copper plate, and the detector with a  $10^{-3}$  rad aperture is placed at angle  $10^{-2}$  rad to the plate surface. The rapid oscillations, parametrized by coefficient  $\nu$  and clearly visible for thin 20 Å film, are caused by the interference of pseudophotons turned away from the electrons at the upper surface and then reflected from both the upper and lower interfaces. This effect is similar to the interference of x rays reflected from different interfaces. The long-period oscillations are governed by the parameter  $\mu$  and are related to the contribution of pseudophotons turned away at the lower interface to the common interference process. The phase difference between both oscillations and their different periodicity follows from the difference in the velocity of photons and pseudophotons. Whereas the photons propagate in the media as light, the velocity of pseudophotons depends on the velocity of electrons. Multiple harmonics, observable in Fig. 4, demonstrate the complexity of the interference process.

The method for calculation of the TR spectrum used in this work and based on the quantum theory of radiation<sup>2</sup> allows us also to take into account the imperfection of interfaces between layers with different refractive indices. To illustrate this feature, let us consider transition radiation from electrons crossing the nonideal boundary between the vacuum and the semi-infinite substrate, i.e., the surface with the profile described by a random function  $z = u(x, y)$ . The nonuniform distribution of the electron density within the plane  $(x, y)$  results in nonconservation of the transverse component of the transfer moment, and formula (1) for spectral-angular distribution of radiation is changed to

$$\frac{\partial^2 N}{\partial \omega \partial \mathbf{n}} = \frac{e^2 \omega}{4\pi^2 c^2} J \left[ 1 - \left( \frac{\mathbf{n}\mathbf{v}}{c} \right)^2 \right] \left\langle \left| \int_{-\infty}^{+\infty} dz \int_S \frac{dx dy}{4\pi^2 S} e^{i[q_z u(x,y) + q_x x + q_y y]} e^{i(p_z - p_{1z})z/\hbar} U_{\mathbf{k}}^{(-)*}(z) \right|^2 \right\rangle. \quad (20)$$

Here the integration in the plane  $(dx, dy)$  is performed over the whole substrate surface  $S$ ; vector  $\mathbf{q} = (\mathbf{p} - \mathbf{p}_1)/\hbar - \mathbf{k}$  defines the moment transfer during the radiation process; the brackets denote the averaging over the statistical distribution of random function  $u(x, y)$ ; and wavefield  $U_{\mathbf{k}}$  describes the solution of Maxwell's equations for an ideal structure. The averaging of the matrix element can be carried out in the same way as in Ref. 19 for the intensity of diffuse x-ray

scattering from rough surface. According to Ref. 19, the root mean square of surface roughness  $\sigma$  and correlation function  $C(x, y)$  are related as

$$\langle [u(x, y) - u(0, 0)]^2 \rangle = 2\sigma^2 - 2C(x, y). \quad (21)$$

Then the distribution of the TR intensity contributing by a rough surface of the sample with permittivity  $\epsilon_f \approx 1$  can be represented as follows:

$$\frac{\partial^2 N}{\partial \omega \partial \mathbf{n}} = \frac{e^2 v^2 \sin^2 \alpha \cos^2 \alpha}{\pi^2 c^2} J \frac{|\epsilon_f - 1|^2}{|\epsilon_f \sin \alpha + \sqrt{\epsilon_f - \cos^2 \alpha}|^2} e^{-q_{0z}^2 \sigma^2} \left( F(\omega, \alpha, 0, 0) + \int \int dq_x dq_y S(q_x, q_y) F(\omega, \alpha, q_x, q_y) \right),$$

$$q_{0z}^2 = k^2 \left( \frac{1}{v^2} - \frac{\sin^2 \alpha}{c^2} \right),$$

$$S(q_x, q_y) = \frac{1}{4\pi^2} \int \int dx dy [e^{q_{0z}^2 C(x,y)} - 1] e^{i(q_x x + q_y y)}, \quad (22)$$

$$F(\omega, \alpha, q_x, q_y) = \left| \frac{1 + 2\delta - \frac{v^2}{c^2} + \frac{v}{c} \sqrt{\epsilon_f - \cos^2 \alpha}}{\left(1 + 2\delta - \frac{v^2}{c^2} \sin^2 \alpha\right) \left(1 + \delta + \frac{v}{c} \sqrt{\epsilon_f - \cos^2 \alpha}\right)} \right|^2,$$

$$\delta = \frac{\hbar c^2 (q_x^2 + q_y^2)}{2\omega E}.$$

The first term in Eq. (22) corresponds to the TR intensity, attenuated due to the Debye-Waller factor, which depends on the longitudinal component of the moment transfer during the photon emission process. The second term is the radiation caused by the correlations in the roughness distribution; it depends on the transverse component of the moment transfer. The expression above demonstrates the fact that TR intensity contains information on surface nonuniformity. However, a detailed investigation of this topic is beyond of the scope of this paper.

#### IV. CONCLUSIONS

In conclusion, the spectra of transition x-ray radiation from nonrelativistic electrons interacting with multilayered structure are described on the basis of the solutions for the uniform Maxwell equations in periodical media. The TR spectrum contains information about the sample that is

analogous to the spatial intensity distribution of the scattered quasimonochromatic x rays, including the information on sample inhomogeneity and imperfections. The advantage of the proposed technique can be realized by a quick measurement of the TR spectral distribution by a fixed detector instead of time-consuming measurement of the spatial reflectivity curves using a goniometer. Both approaches can supplement each other in nanotechnology test instruments, combining the detailed information delivered by angular reflectivity measurements and time-saving spectral measurements of transition radiation. Three typical examples of structures, viz., single substrate, superlattice on a substrate, and thin plate, are used for an illustration of the main features of specular and Bragg reflections of x rays produced by electrons. The applicable range of wavelengths for the observation of TR with a background of incoherent bremsstrahlung has been discussed.

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<sup>1</sup>M. L. Ter-Mikaelian, *High Energy Electromagnetic Processes in Condensed Media* (Wiley, New York, 1972).

<sup>2</sup>V. G. Baryshevskii and I. D. Feranchuk, *J. Phys. (Paris)* **44**, 913 (1983).

<sup>3</sup>I. D. Feranchuk and A. Ulyanenkov, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **55**, 466 (1999).

<sup>4</sup>I. D. Feranchuk, A. Ulyanenkov, J. Harada, and J. C. H. Spence, *Phys. Rev. E* **62**, 4225 (2000).

<sup>5</sup>V. V. Morokhovskiy, J. Freudenberger, H. Genz, V. L. Morokhovskii, A. Richter, and J. P. F. Sellschop, *Phys. Rev. B* **61**, 3347 (2000).

<sup>6</sup>A. P. Potylitsyn, P. V. Karataev, and G. A. Naumenko, *Phys. Rev. E* **61**, 7039 (2000).

<sup>7</sup>B. Lastdrager, A. Tip, and J. Verhoeven, *Phys. Rev. E* **61**, 5767 (2000).

<sup>8</sup>Y. Takahura and O. Haerberle, *Phys. Rev. E* **61**, 4441 (2000).

<sup>9</sup>I. F. Frank and V. L. Ginzburg, *J. Phys. (Moscow)* **9**, 353 (1945).

<sup>10</sup>N. V. Smith and D. P. Woodruff, *Prog. Surf. Sci.* **21**, 295 (1986).

<sup>11</sup>G. Borstel and G. Thörner, *Surf. Sci. Rep.* **8**, 3 (1988).

<sup>12</sup>R. W. James, *The Optical Principles of the Diffraction of X-Rays* (Ox Bow Press, Connecticut, 1982).

<sup>13</sup>V. E. Pafomov, *Zh. Tekh. Fiz.* **33**, 557 (1963) [*Sov. Phys. Tech. Phys.* **8**, 412 (1963)]; *Proc. Lebedev Inst. of Physics* **44**, 25 (1971).

<sup>14</sup>V. Holý, U. Pietsch, and T. Baumbach, *X-ray Scattering by Thin Films and Multilayers* (Springer-Verlag, Berlin, 1998).

<sup>15</sup>L. G. Parratt, *Phys. Rev.* **95**, 359 (1954).

<sup>16</sup>V. G. Baryshevsky and I. D. Feranchuk, *Izv. Belaruss. Akad. Sci. Ser. Fiz.-Mat. Nauk* **2**, 117 (1975).

<sup>17</sup>V. L. Ginzburg, *Theoretical Physics and Astrophysics* (Nauka, Moscow, 1975).

<sup>18</sup>W. Koch and J. W. Motz, *Rev. Mod. Phys.* **31**, 920 (1961).

<sup>19</sup>S. K. Sinha, E. B. Sirota, S. Garoff, and H. B. Stanley, *Phys. Rev. B* **38**, 2297 (1988).