

A

Appendix

A.1 X-ray Polarizability and Eigenwaves for the Electromagnetic Field in a Crystal

The general expression for the tensor of the dielectric permittivity $\epsilon_{ij}(\mathbf{k}, \mathbf{k}_g, \omega)$ in the constitutive equation (2.4) contains the tensor of the X-ray polarizability χ_{ij} , which describes the interaction of X-ray radiation with the crystal:

$$\epsilon_{ij}(\mathbf{k}, \mathbf{k}_g, \omega) = \delta_{ij} \delta_{\mathbf{k}, \mathbf{k}_g} + \chi_{ij}(\mathbf{k}, \mathbf{k}_g, \omega), \quad i, j = 1, 2, 3. \quad (\text{A.1})$$

The components of χ_{ij} are not phenomenological parameters but microscopic characteristics of the crystal, which are expressed through the amplitudes of the scattering of X-ray photons on periodically arranged atoms and nuclei (see, for example, [6]):

$$\chi_{ij}(\mathbf{k}, \mathbf{k}_g, \omega) = \frac{4\pi c^2}{\omega^2 \Omega} \sum_a \left[f_{ij,a}^{(e)}(\mathbf{g}, \omega) + f_{ij,a}^{(n)}(\mathbf{k}, \mathbf{k}_g, \omega) \right] e^{i\mathbf{g}R_a}. \quad (\text{A.2})$$

Here Ω is the volume of a crystallographic unit cell; R_a is the coordinate of the a th atom in the cell; $f_{ij,a}^{(e)}$ is the amplitude of the elastic coherent scattering of photons on atom's electrons [8]:

$$f_{ij,a}^{(e)}(\mathbf{g}, \omega) = -\delta_{ij} r_0 [F_a(\mathbf{g}) + \Delta f'_a(\omega) + i\Delta f''_a(\omega)] e^{-W_a(\mathbf{g})}, \quad (\text{A.3})$$

where $r_0 = e^2/mc^2$ is the electromagnetic radius of an electron; $F_a(\mathbf{g})$ is an atomic scattering factor; $\Delta f'_a(\omega)$, $\Delta f''_a(\omega)$ are the real and imaginary parts of anomalous dispersion corrections, respectively, which take into account the absorption and resonant scattering of photons; $e^{-W_a(\mathbf{g})}$ is the Debye–Waller factor, which quantifies the reduction of the elastic amplitude due to inelastic scattering on the crystal phonons. The method for calculation of the X-ray polarizability for various crystals is presented in [7].

The contribution to polarizability by the scattering of photons on resonant nuclear transitions is essential for Mössbauer crystals [1]:

$$f_{ij,a}^{(n)}(\mathbf{k}, \mathbf{k}_g, \omega) = -\frac{\tilde{n}}{4\omega_r} \frac{2J+1}{2J_0+1} \frac{\Gamma_1}{\hbar(\omega - \omega_r) + \Gamma} P_{ij}(\mathbf{k}, \mathbf{k}_g) \eta_a e^{-W_a(\mathbf{k}, \mathbf{k}_g)}. \quad (\text{A.4})$$

where ω_r is the frequency of resonant transition of nuclei of the cell with weight η_a ; Γ_1 and Γ are the elastic and total widths of the excited level, respectively; J_1 and J are the angular moments of the excited and ground states, respectively; the polarization factor $P_{ij}(\mathbf{k}, \mathbf{k}_g)$ is determined by the multiplicity of transition:

$$\begin{aligned} E1 \rightarrow P_{ij} &= \delta_{ij}, & M1 \rightarrow P_{ij} &= \frac{(\mathbf{k}\mathbf{k}_g)\delta_{ij} - k_i k_{gj}}{k^2}, \\ E2 \rightarrow P_{ij} &= \frac{1}{k^2} [(\mathbf{k}\mathbf{k}_g)\delta_{ij} + k_j k_{gi} - 2k_i k_{gj}]. \end{aligned}$$

The Debye–Waller factor depends on the ratio of the width Γ to the phonon energy of a crystal $\hbar\omega_{\text{phon}}$:

$$\begin{aligned} W_a(\mathbf{k}, \mathbf{k}_g) &= \frac{1}{2} \overline{u_a^2} (k^2 + k_g^2), & \Gamma &\ll \hbar\omega_{\text{phon}}, \\ W_a(\mathbf{k}, \mathbf{k}_g) &= \frac{1}{2} \overline{u_a^2} g^2, & \Gamma &\gg \hbar\omega_{\text{phon}}, \end{aligned}$$

where $\overline{u_a^2}$ is the mean square amplitude of nuclear oscillations near an equilibrium position.

In the X-ray domain, the X-ray polarizability is typically $|\chi_{i,j}| \sim 10^{-4} - 10^{-6}$. For the solution of Maxwell's equations (2.1) with the accuracy $O(|\chi_{i,j}|^2)$, the electromagnetic field in a medium remains transverse, and the interaction between the field and the crystal is essential at the wave vectors \mathbf{k} , satisfying the Bragg condition [9]:

$$\alpha_B = \frac{2\mathbf{k}\mathbf{g} + g^2}{k^2} \leq \chi_0. \quad (\text{A.5})$$

In most cases, condition (A.5) is fulfilled for only one reciprocal lattice vector \mathbf{g} for fixed \mathbf{k} , and the two-wave approximation of the dynamical diffraction theory is valid [3]. Then, the eigenwaves of the electromagnetic field, required for description of processes in the crystal (Sect. 3.2), are composed of the linear combination of plane waves:

$$\begin{aligned} \mathbf{A}_{\mathbf{k}\omega}^{(s)}(\mathbf{r}) &= \mathbf{e}_s A_{ks} e^{i\mathbf{k}\mathbf{r}} + \mathbf{e}_{gs} A_{gs} e^{i\mathbf{k}_g\mathbf{r}}, & s &= \sigma, \pi, \\ \mathbf{E}_{\mathbf{k}\omega}^{(s)}(\mathbf{r}) &= i \frac{\omega}{c} \mathbf{A}_{\mathbf{k}\omega}^{(s)}(\mathbf{r}), \end{aligned} \quad (\text{A.6})$$

where the unit polarization vectors are

$$\mathbf{e}_\sigma \parallel \mathbf{e}_{g\sigma} \parallel [\mathbf{k} \times \mathbf{g}], \quad \mathbf{e}_\pi \parallel [\mathbf{k} \times [\mathbf{k} \times \mathbf{g}]], \quad \mathbf{e}_{g\pi} \parallel [\mathbf{k}_g \times [\mathbf{k} \times \mathbf{g}]],$$

and the amplitudes of wave (A.6) have to satisfy the algebraic equations:

$$\begin{aligned}
& \{k^2 - k_0^2(1 + \chi_{00}^{(s)})\}A_{ks} - k_0^2\chi_{01}^{(s)}A_{gs} = 0, \\
& \{k_g^2 - k_0^2(1 + \chi_{11}^{(s)})\}A_{gs} - k_0^2\chi_{10}^{(s)}A_{ks} = 0, \\
& k_0 = \frac{\omega}{c}, \quad \chi_{00}^{(s)} = e_{si}e_{sj}\chi_{ij}(\mathbf{k}, \mathbf{k}), \quad \chi_{11}^{(s)} = e_{gsi}e_{gsj}\chi_{ij}(\mathbf{k}_g, \mathbf{k}_g), \\
& \chi_{01}^{(s)} = e_{si}e_{gsj}\chi_{ij}(\mathbf{k}, \mathbf{k}_g), \quad \chi_{10}^{(s)} = e_{gsi}e_{sj}\chi_{ij}(\mathbf{k}_g, \mathbf{k}). \quad (\text{A.7})
\end{aligned}$$

If the resonant scattering of X-rays on atoms and nuclei is negligible, then

$$\begin{aligned}
\chi_{00}^{(s)} = \chi_{11}^{(s)} = \chi_0, \quad \chi_{01}^{(s)} = \chi_{-g}C_s, \quad \chi_{10}^{(s)} = \chi_gC_s, \\
C_\sigma = 1, \quad C_\pi = \cos 2\theta_B.
\end{aligned}$$

The condition of zero determinant for system (A.7) delivers the effective refraction indices for eigenwaves inside a crystal:

$$\begin{aligned}
\mathbf{k}_{\mu s} = k_0 \frac{\mathbf{k}}{k} n_{\mu s}, \quad n_{\mu s}(1 + \epsilon_{\mu 1}), \quad \mu = 1, 2, \\
\epsilon_{\mu s} = \frac{1}{4} \left[q \pm \sqrt{q^2 + 4\beta\chi_{00}\alpha_B - \chi_{00}\chi_{11} + \chi_{01}^{(s)}\chi_{10}^{(s)}} \right], \\
q = \chi_{00} + \beta\chi_{11} - \beta\alpha_B, \quad \beta = \frac{\gamma_0}{\gamma_g}, \quad \gamma_0 = \cos(\mathbf{k}, \mathbf{N}), \quad \gamma_g = \cos(\mathbf{k}_g, \mathbf{N}), \quad (\text{A.8})
\end{aligned}$$

where \mathbf{N} is a normal to the crystal surface.

A.2 Asymptotic for the Green Function and Boundary Conditions for the Electromagnetic Field

The asymptotic of the Green function (Sect. 2.1) for Maxwell's equations in the medium with an arbitrary dielectric permittivity is derived here in the limit $r \gg r'$. This function is the solution of the following equation ($k_0 = \omega/c$, $\alpha, \beta = 1, 2, 3$):

$$\begin{aligned}
\epsilon_{\alpha\beta\gamma}\epsilon_{\gamma\mu\nu} \frac{\partial^2}{\partial x_\beta \partial x_\mu} G_{\nu\lambda}(\mathbf{r}, \mathbf{r}', \omega) - k_0^2 \int d\mathbf{r}_1 \epsilon_{\alpha\beta}(\mathbf{r}, \mathbf{r}_1, \omega) G_{\beta\lambda}(\mathbf{r}_1, \mathbf{r}', \omega) \\
= \delta_{\alpha\lambda} \delta(\mathbf{r} - \mathbf{r}'). \quad (\text{A.9})
\end{aligned}$$

Expressing the dielectric permittivity through the X-ray polarizability

$$\epsilon_{\alpha\beta}(\mathbf{r}, \mathbf{r}_1, \omega) = \delta_{\alpha\beta} \delta(\mathbf{r} - \mathbf{r}_1) + \chi_{\alpha\beta}(\mathbf{r}, \mathbf{r}_1, \omega),$$

Equation (A.9) is reformulated in the integral form:

$$\begin{aligned}
G_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega) = G_{\alpha\beta}^{(0)}(\mathbf{r}, \mathbf{r}', \omega) \\
+ k_0^2 \int d\mathbf{r}_1 d\mathbf{r}_2 G_{\alpha\mu}^{(0)}(\mathbf{r}, \mathbf{r}_1, \omega) \chi_{\mu\nu}(\mathbf{r}_1, \mathbf{r}_2, \omega) G_{\nu\beta}(\mathbf{r}_2, \mathbf{r}', \omega). \quad (\text{A.10})
\end{aligned}$$

The Green function $G_{\alpha\beta}^{(0)}(\mathbf{r}, \mathbf{r}', \omega)$ for equation (A.9) in vacuum is represented [12] as an expansion of eigenstates of the free electromagnetic field:

$$G_{\alpha\beta}^{(0)}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{(2\pi)^3} \int d\mathbf{q} \sum_{s=1,2} \frac{e_{\alpha}^{(s)}(\mathbf{q})e_{\beta}^{(s)*}(\mathbf{q})e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')}}{q^2 - k_0^2(1+iO)}, \quad (\text{A.11})$$

where $e^{(s)}(\mathbf{q})$, $s = 1, 2$; $(\mathbf{q}, \mathbf{e}^{(s)}) = 0$ are two mutually orthogonal unit vectors of polarization of the plane electromagnetic wave with the wave vector \mathbf{q} . In the considered case here, $r \gg r'$, the following asymptotic for the function $G_{\alpha\beta}^{(0)}$ is valid:

$$G_{\alpha\beta}^{(0)}(\mathbf{r}, \mathbf{r}', \omega) \approx \frac{1}{4\pi} \sum_{s=1,2} e_{\alpha}^{(s)}(\mathbf{k})e_{\beta}^{(s)*}(\mathbf{k}) \frac{e^{ik_0r}}{r} e^{-i\mathbf{k}\mathbf{r}'}, \quad \mathbf{k} = k_0 \frac{\mathbf{r}}{r}. \quad (\text{A.12})$$

Using (A.12), the asymptotic (A.10) can be written as

$$G_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega) \approx \frac{1}{4\pi} \frac{e^{ik_0r}}{r} \sum_{s=1,2} e_{\alpha}^{(s)}(\mathbf{k}) \times \left[e_{\beta}^{(s)}(\mathbf{k})e^{i\mathbf{k}\mathbf{r}'} + k_0^2 \int d\mathbf{r}_1 d\mathbf{r}_2 e^{i\mathbf{k}\mathbf{r}_1} \chi_{\mu\nu}^*(\mathbf{r}_1, \mathbf{r}_2, \omega) G_{\nu\beta}^*(\mathbf{r}_2, \mathbf{r}', \omega) \right]^*. \quad (\text{A.13})$$

If the iterative solution of (A.10) for the exact Green function is used, the expression in the square brackets in (A.13) is represented as the series

$$E_{\mathbf{k},\beta}^{(s,-)}(\mathbf{r}) = e_{\beta}^{(s)}(\mathbf{k})e^{i\mathbf{k}\mathbf{r}} + k_0^2 \int d\mathbf{r}_1 d\mathbf{r}_2 G_{\nu\mu}^{(0,*)}(\mathbf{r}, \mathbf{r}_1, \omega) \chi_{\beta\nu}^*(\mathbf{r}_1, \mathbf{r}_2, \omega) e_{\mu}^{(s)}e^{i\mathbf{k}\mathbf{r}_2} + \dots, \quad (\text{A.14})$$

where the asymptotic behaviour of the function

$$G_{\alpha\beta}^{(0,*)}(\mathbf{r}, \mathbf{r}', \omega) \approx \frac{1}{4\pi} \sum_{s=1,2} e_{\alpha}^{(s)*}(\mathbf{k})e_{\beta}^{(s)}(\mathbf{k}) \frac{e^{-ik_0r}}{r} e^{i\mathbf{k}\mathbf{r}'}$$

corresponds to a convergent spherical wave.

We now consider the eigenstates of the electromagnetic field in the medium with the dielectric permittivity $\epsilon_{\alpha\beta}^*(\mathbf{r}, \mathbf{r}_1, \omega)$, which are the solutions of the homogeneous equation analogous to (A.9):

$$\epsilon_{\alpha\beta\nu} \epsilon_{\nu\mu\gamma} \frac{\partial^2}{\partial x_{\beta} \partial x_{\mu}} E_{\mathbf{k},\gamma}^{(s,-)} - k_0^2 \int d\mathbf{r}_1 \epsilon_{\alpha\beta}^*(\mathbf{r}, \mathbf{r}_1, \omega) E_{\mathbf{k},\beta}^{(s,-)} = 0. \quad (\text{A.15})$$

The integral form of this equation, after using the Green function $G_{\alpha\beta}^{(0,*)}(\mathbf{r}, \mathbf{r}', \omega)$ and normalizing to the unit amplitude of the incident wave, is

$$E_{\mathbf{k},\alpha}^{(s,-)}(\mathbf{r}) = e_{\alpha}^{(s)}(\mathbf{k})e^{i\mathbf{k}\mathbf{r}} + k_0^2 \int d\mathbf{r}_1 d\mathbf{r}_2 G_{\alpha\beta}^{(0,*)}(\mathbf{r}, \mathbf{r}_1, \omega) \chi_{\beta\gamma}^*(\mathbf{r}_1, \mathbf{r}_2, \omega) E_{\mathbf{k},\beta}^{(s,-)}(\mathbf{r}_2) = 0, \quad (\text{A.16})$$

and the iterative solution of this equation is delivered by series (A.15), which confirms (2.11) in Sect. 2.1.

The matrix elements for amplitudes of the electromagnetic field in the crystal are calculated (see Sect. 3.1) on the basis of the vector potential $\mathbf{A}_{\mathbf{k}}^{(s,-)}(\mathbf{r})$ and boundary conditions at the entrance and exit surfaces of the sample. The conventional boundary conditions of electrodynamics (the continuity of the tangential component of the field strength vectors and the normal components of the induction vectors [10]) in the X-ray region are reduced [9] with the accuracy $O(|\chi_0|^2)$ to the continuity of all field components and their derivatives. Within the framework of the two-wave approximation for the dynamical diffraction theory, (A.6)–(A.8) have to be taken into account. Then, the normalized vector potential, which is continuous at the sample surfaces $z = 0$ and $z = L$, is (see 3.14)

$$\mathbf{A}_{\mathbf{k}}^{(s,-)}(\mathbf{r}) = \sqrt{4\pi} e^{i\mathbf{k}\mathbf{r}} \{ \mathbf{e}_s \Phi^{(s)}(z) + \mathbf{e}_{gs} \Phi_g^{(s)}(z) e^{ig\mathbf{r}} \}. \quad (\text{A.17})$$

The explicit expressions for $\Phi^{(s)}(z)$ and $\Phi_g^{(s)}(z)$ in the case of different diffraction geometries and photon observation angles are as follows:

(1a) The Bragg case ($\beta < 0$, $\gamma_0 > 0$, $\gamma_g < 0$):

$$\begin{aligned} \Phi^{(s)}(z) &= \{ D_{s0}^*(0)H(-z) + D_{s0}^*(z)H(z)H(L-z) + H(z-L) \} e^{-ik_z L}, \\ \Phi_g^{(s)}(z) &= \beta \xi_s^{g*} \{ D_{sg}^*(z)H(z)H(L-z) + D_{sg}^*(L)H(z-L) \} e^{-ik_z L}, \\ D_{s0}(z) &= \xi_{1s}^0 e^{-ik_0 \epsilon_{1s} z / \gamma_0} + \xi_{2s}^0 e^{-ik_0 \epsilon_{2s} z / \gamma_0}, \\ D_{sg}(z) &= e^{-ik_0 \epsilon_{1s} z / \gamma_0} - e^{-ik_0 \epsilon_{2s} z / \gamma_0}, \\ \xi_{1,2s}^0 &= \pm \frac{2\epsilon_{2,1s} - \chi_{00}}{\Delta_s}, \quad \xi_s^g = \frac{\chi_{10}^s}{\Delta_s}, \\ \Delta_s &= (2\epsilon_{2s} - \chi_{00})e^{-ik_0 \epsilon_{1s} z / \gamma_0} - (2\epsilon_{1s} - \chi_{00})e^{-ik_0 \epsilon_{2s} z / \gamma_0}. \end{aligned} \quad (\text{A.18})$$

(1b) The Bragg case ($\beta < 0$, $\gamma_0 < 0$, $\gamma_g > 0$):

$$\begin{aligned} \Phi^{(s)}(z) &= H(-z) + D_{s0}^{(1*)}(z)H(z)H(L-z) + D_{s1}^{(1*)}(L)H(z-L), \\ \Phi_g^{(s)}(z) &= -\beta \xi_s^{g*} \left\{ D_{sg}^{(1*)}(0)H(-z) + D_{sg}^{(1*)}(z)H(z)H(L-z) \right\}, \\ D_{s0}^{(1)}(z) &= \xi_{1s}^0 e^{ik_0(\epsilon_{1s}z + \epsilon_{2s}L)/|\gamma_0|} + \xi_{2s}^0 e^{ik_0(\epsilon_{2s}z + \epsilon_{1s}L)/|\gamma_0|}, \\ D_{sg}^{(1)}(z) &= e^{ik_0(\epsilon_{1s}z + \epsilon_{2s}L)/|\gamma_0|} - e^{ik_0(\epsilon_{2s}z + \epsilon_{1s}L)/|\gamma_0|}. \end{aligned} \quad (\text{A.19})$$

(2a) The Laue case ($\beta > 0$, $\gamma_0 > 0$, $\gamma_g > 0$):

$$\begin{aligned}
\Phi^{(s)}(z) &= D_{s0}^{(2*)}(L)H(-z) + D_{s0}^{(2*)}(L-z)H(z)H(L-z) \\
&\quad + e^{-ik_z L}H(z-L), \\
\Phi_g^{(s)}(z) &= \beta \left\{ D_{sg}^{(2*)}(L)H(-z) + D_{sg}^{(2*)}(L-z)H(z)H(L-z) \right\}, \\
D_{s0}^{(2)}(z) &= -\zeta_{1s}^0 e^{ik_0 \epsilon_{1s} z / \gamma_0} - \zeta_{2s}^0 e^{ik_0 \epsilon_{2s} z / \gamma_0}, \\
D_{sg}^{(2)}(z) &= \zeta_{1s}^g e^{ik_0 \epsilon_{1s} z / \gamma_0} + \zeta_{2s}^0 e^{ik_0 \epsilon_{2s} z / \gamma_0}, \\
\zeta_{1,2s}^0 &= \mp \frac{2\epsilon_{2,1s} - \chi_{00}}{2(\epsilon_{2s} - \epsilon_{1s})}, \quad \zeta_{1,2s}^g = \mp \frac{\chi_{01}^s}{2(\epsilon_{2s} - \epsilon_{1s})}. \tag{A.20}
\end{aligned}$$

(2b) The Laue case ($\beta > 0$, $\gamma_0 < 0$, $\gamma_g < 0$):

$$\begin{aligned}
\Phi^{(s)}(z) &= H(-z) + D_{s0}^{(3*)}(z)H(z)H(L-z) + D_{s0}^{(3*)}(L)H(z-L), \\
\Phi_g^{(s)}(z) &= \beta \left\{ D_{sg}^{(3*)}(z)H(z)H(L-z) + D_{sg}^{(3*)}(L-z)H(z-L) \right\}, \\
D_{s0}^{(3)}(z) &= -\zeta_{1s}^0 e^{ik_0 \epsilon_{1s} z / |\gamma_0|} - \zeta_{2s}^0 e^{ik_0 \epsilon_{2s} z / |\gamma_0|}, \\
D_{sg}^{(3)}(z) &= \zeta_{1s}^g e^{ik_0 \epsilon_{1s} z / |\gamma_0|} - \zeta_{2s}^0 e^{ik_0 \epsilon_{2s} z / |\gamma_0|}. \tag{A.21}
\end{aligned}$$

A.3 Accurate Calculation of PXR with Multiple Scattering of Electrons

For the description of PXR fine structure and high-resolution PXR, a more accurate calculation than that in Sect. 2.3 of the multiple scattering of charged particles is necessary. Equation (2.16) has to be averaged over all the particle trajectories in the crystal [4, 5]:

$$\begin{aligned}
W_{n\omega}^{(s)} &= \frac{q^2 \omega^2}{4\pi^2 c^3} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' w_1(\mathbf{r}, \mathbf{v}, t) w_2(\mathbf{r}, \mathbf{v}, t | \mathbf{r}', \mathbf{v}', t') \\
&\quad e^{i\omega(t-t')} \left(\mathbf{v} \mathbf{E}_{\mathbf{k}s}^{(-)}(\mathbf{r}, \omega) \right)^* \left(\mathbf{v}' \mathbf{E}_{\mathbf{k}s}^{(-)}(\mathbf{r}', \omega) \right), \tag{A.22}
\end{aligned}$$

where $w_1(\mathbf{r}, \mathbf{v}, t)$ is the particle distribution function at the time t , $w_2(\mathbf{r}, \mathbf{v}, t | \mathbf{r}', \mathbf{v}', t')$ is the probability density to find a particle at the time t' at the position \mathbf{r}', \mathbf{v}' , if it was at the position \mathbf{r}, \mathbf{v} at the time t .

The periodic crystal structure influences the beam distribution function in a small phase volume near the boundaries of the Brillouin zones. This case is essential if the primary beam velocity \mathbf{v}_0 is parallel to the crystallographic axes (planes) and particles are trapped into the channelling mode. In other cases, the kinetic equation for a homogeneous medium can be used for averaging the distribution function over the trajectories. The energy E and ϑ of velocity deviation are more convenient variables to be used in w_1, w_2 instead of the velocity \mathbf{v} . In the case of relativistic particles $\vartheta \ll 1$, the kinetic equation is [4]

$$\begin{aligned}
\frac{\partial w}{\partial t} + \mathbf{v} \frac{\partial w}{\partial \mathbf{r}} &= q(E) \Delta_{\vartheta} w + \hat{K}(E) w ; \\
q(E) &= \frac{c}{L_R} \frac{E_s^2}{4E^2}, \quad \Delta_{\vartheta} = \frac{\partial^2}{\partial \vartheta_x^2} + \frac{\partial^2}{\partial \vartheta_y^2}, \\
\hat{K}(E) w &= \int_0^{\infty} \frac{u^2 + E^2 - 2uE/3}{(u - E)} \left[\frac{w(\vartheta, u, t)}{u^2} H(u - E) \right. \\
&\quad \left. + \frac{w(\vartheta, E, t)}{E^2} H(E - u) \right]. \tag{A.23}
\end{aligned}$$

Equation (A.23) uses the Bete–Gaitler [2] formula for bremsstrahlung, which is dominant in particle energy losses; the parameter E_s and L_R from (1.26) are the characteristic energy and the radiation length of the multiple scattering of electron beam on the shielded potential of crystal atoms, respectively. The functions w_1 and w_2 are the solutions of (A.23) under different initial conditions:

$$\begin{aligned}
w_1(t = 0) &= \delta(\mathbf{r} - \mathbf{r}_0) \delta(\vartheta_x) \delta(\vartheta_y) \delta(E - E_0), \\
w_2(t = t') &= \delta(\mathbf{r} - \mathbf{r}') \delta(\vartheta_x - \vartheta'_x) \delta(\vartheta_y - \vartheta'_y) \delta(E - E'), \tag{A.24}
\end{aligned}$$

where \mathbf{r}_0 and E_0 are the initial position and the beam energy at the time $t = 0$, respectively.

To analyse the radiation spectrum in a crystal of thickness L , the expressions for wave fields from Appendix A.2 have to be used. The integration area is divided into three parts: $(-\infty, 0)$, $(0, t_0)$, (t_0, ∞) , where $t_0 = L/(\mathbf{v}_0 \mathbf{N})$ corresponds to the time of the escape of the particle from the crystal and the fluctuations of the time taken by the particle to pass through the crystal due to multiple scattering are neglected; \mathbf{N} is a normal to the crystal surface. Thus, there are nine different contributions to the total radiation intensity, each having a certain physical interpretation and depending on the experimental geometry. The detailed analysis of (A.22) is given in [5], and an example of the Laue geometry is presented below. For relativistic particles, the energy losses for radiation are comparatively low, whereas multiple scattering is essential. Then the operator $\hat{K}(E)$ in (A.23) can be dropped and $q(E) = q(E_0) \equiv q_0$ is constant, and the solution of (A.23) for $w_1(\mathbf{r}, \vartheta, t)$, $w_2(\mathbf{r} - \mathbf{r}', \vartheta, \vartheta', t - t')$ with the initial conditions (A.24) are derived in [13, 14]. The contribution to the intensity (A.22) due to the particle trajectory in the crystal is [5]

$$\begin{aligned}
W_{\mathbf{n}\omega}^{(s)} &= \frac{q^2 \omega^2}{2\pi^2 c^3} C_s^2 \left| \frac{\chi_g}{2(\epsilon_{2s} - \epsilon_{1s})} \right|^2 \operatorname{Re} \int_0^{t_0} dt \int_0^{t_0-t} d\tau \\
&\quad \times [(\mathbf{e}_{gs} \mathbf{v}_0)^2 Q_1(1 + \Delta) + 2q_0 t Q_2] \left[\sum_{\mu=1,2} F_{\mu s} - \Phi_s \right], \tag{A.25}
\end{aligned}$$

where the polarization factor C_s and the diffraction parameters follow from A.2, and the multiple scattering is determined by

$$\begin{aligned}
Q_1 &= \frac{1}{\cosh u(1 + \eta\tau \tanh u)} \exp \left[\frac{i\omega\tau\theta^2}{2} - \frac{\eta\theta^2 \tanh u}{4q(1 + \eta\tau \tanh u)} \right], \\
Q_2 &= \frac{Q_1}{\cosh u(1 + \eta\tau \tanh u)}, \quad \Delta = \frac{1 - \cosh u(1 + \eta\tau \tanh u)^2}{\cosh u(1 + \eta\tau \tanh u)^2}, \\
F_{\mu s} &= \exp \left[-\frac{ic\tau}{L_{\mu s}} - \frac{t_0 - t - \tau/2}{L_{\mu s}^{(a)}} \right], \\
\Phi_s &= \exp \left[-\frac{ic\tau}{L_{2s}} + \frac{\tau}{L_{2s}^{(a)}} - i\omega(\epsilon_{2s}^* - \epsilon_{1s})(t_0 - t) \right] \\
&+ \exp \left[-\frac{ic\tau}{L_{2s}} - \frac{\tau}{L_{2s}^{(a)}} + i\omega(\epsilon_{2s} - \epsilon_{1s}^*)t \right], \\
u &= \eta\tau, \quad \eta = \sqrt{2i\omega q_0}, \\
L_{\mu s} &= \frac{2c}{\omega[\gamma^{-2} + \theta^2 + 2(1 - \operatorname{Re} \epsilon_{\mu s})]}, \quad L_{\mu s}^{(a)} = \frac{2c}{\omega \operatorname{Im} \epsilon_{\mu s}}. \quad (\text{A.26})
\end{aligned}$$

The functions Q_1 , Q_2 and Δ depend on the coherent length of bremsstrahlung [14]:

$$L_{\text{BS}} = \frac{c}{\sqrt{2\omega q_0}},$$

and their influence on the spectral-angular characteristics of radiation is determined by the ratio of L_{BS} and PXR coherent length $L_{\mu s}$.

For high-energy electrons ($L_{\text{BS}} \sim \gamma \rightarrow \infty$) or for heavy charged particles ($q_0 \rightarrow 0$), the functions $Q_{1,2} \rightarrow 1$, $\Delta \rightarrow 0$. Then the main contribution to the intensity is given by the first term in (A.25), which has a minimum $\sim \theta^2$ of the photon radiation in the diffraction direction \mathbf{k}_B . The term in (A.25) proportional to $2q_0 t Q_2$ corresponds to bremsstrahlung, which has a maximum in the direction \mathbf{k}_B . In the case of thin crystals, these facts fit well the results of Sect. 2.3. In general, the influence of multiple scattering results in cumbersome expressions and has been investigated in [5]. Here we emphasize only the expression which is useful for fitting of the HRPXR experimental data (see Sect. 2.3). The formula used in (3.26) for the photon radiation angle,

$$\theta_{\text{ph}}^2 = \gamma^{-2} + \theta_{\text{sc}}^2 + \theta_{\text{M}}^2,$$

has to be substituted for higher accuracy by

$$\theta_{\text{ph}}^2 = \gamma^{-2} + \zeta\theta_{\text{sc}}^2 + \theta_{\text{M}}^2,$$

and the dimensionless parameter ζ is varied in the region $1.2 < \zeta < 3$ for different crystal thicknesses [5].

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