Polarization bremsstrahlung study of short-range order in solids

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A B S T R A C T

Possibility to elaborate a new method of the diagnostics of short range order in solids based on spectral measurements of polarization bremsstrahlung from relativistic electrons moving in a sample is shown. The main advantage of the method being proposed consists in the absence of distortions in desired function of atom radial density in distinction to that determined by the basic Zernicke–Prins approach based on angular measurements of scattered quasi-monochromatic X-rays.

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1. Introduction

When a fast charged particle moves in a medium it can emit electromagnetic waves due to the scattering of particle Coulomb field by electrons of medium atoms. This emission mechanism additional to the ordinary bremsstrahlung is known as the polarization bremsstrahlung (PB) [1]. Such properties of PB as a large value of effective impact parameters in the collision with an atom comparable with the atomic size and well-determined spectrum of virtual photons associated with projectile Coulomb field are of interest in the field of solid structure diagnostics on the base of EDXD (energy dispersive X-ray diffraction) approach [2]. The variant of EDXD being discussed is of immediate interest to develop the method of structure diagnostics with high space resolution. Indeed, the problem of a primary electron beam focusing on the sample by equipments of an ordinary magnetic optics is incomparably less than that for X-ray beam. Experiments [3,4] have demonstrated that PB is candidate for polycrystalline structure diagnostics. The aim of our work is to show the basic possibility to use PB for a measurement of radial density of atoms in amorphous and ordered in part media. We show that a necessary condition for effective measurements consists in the use of PB photons emitted in backward direction relative to an emitting electron velocity. It is interesting to note in this connection that backward PB is best suited to determine a polycrystalline structure as well [5]. The system of units $\hbar = c = 1$ is used in the work.

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2. Let us consider the spectral–angular characteristics of PB photons emitted by relativistic electrons crossing a thin solid target starting from Maxwell equation for Fourier transform of excited electric field

$$\left(k^2 - \omega^2\right)\mathbf{E}_{\omega\mathbf{k}} - \mathbf{k}(\mathbf{k}\cdot\mathbf{E}_{\omega\mathbf{k}}) = 4\pi i\omega\mathbf{J}_{\omega\mathbf{k}} + \frac{i\omega e}{2\pi^2}\mathbf{V}\delta(\omega - \mathbf{k}\cdot\mathbf{V}). \quad (1)$$

Here the last item in the right side of (1) describes the current density of a fast electron, $\mathbf{J}$ is the induced current density of medium electrons, determined within the frame of dipole approximation by the equations:

$$4\pi i\omega\mathbf{J}_{\omega\mathbf{k}} = \omega^2 \int d^3k'\, G\left(\mathbf{k}' - \mathbf{k}\right)\mathbf{E}_{\omega\mathbf{k}'},$$

$$G = \frac{1}{2\pi^2}\frac{\alpha_0(\omega)}{1 + (\mathbf{k}' - \mathbf{k})^2 R^2}\sum_l e^{i(\mathbf{k}' - \mathbf{k})\mathbf{r}_l},$$

$$\alpha_0 = \frac{e^2}{m}\sum_{n\geq 1}\frac{f_{n0}}{\omega_{n0}^2 - \omega^2}, \quad (2)$$

where R is the screening radius in Fermi–Thomas atom model (the simplest model with exponential screening is used in our calculations), summation in (2) is performed over all atoms in the target, $\mathbf{r}_l$ is the coordinate of l-th atom, $\alpha_0(\omega)$ is the ordinary dipole polarizability of an atom.

The function G describes both refraction and scattering of photons in the target. It is convenient for the further analysis to sep-

arate G into averaged over coordinates of all atoms and accidental components

$$G = \bar{G} + \tilde{G}, \qquad \bar{G} = \langle G \rangle = 4\pi n_0 \alpha_0(\omega)\delta(\mathbf{k}' - \mathbf{k}),$$
$$4\pi n_0 \alpha_0(\omega) = \chi(\omega), \qquad 1 + \chi(\omega) = \varepsilon(\omega), \tag{3}$$

so that the scattering of a fast electron Coulomb field will be described by $\tilde{G}$ only. Here n_0 is the average density of atoms, $\chi(\omega)$ and $\varepsilon(\omega)$ are the dielectric susceptibility and permeability of the target respectively.

The solution of (1) should be determined by perturbation theory. Substituting (3) into (1) and representing the total field $\mathbf{E}_{\omega\mathbf{k}}$ as a sum of the electron Coulomb field $\mathbf{E}^{eq}_{\omega\mathbf{k}}$ and the emission field $\mathbf{E}^{rad}_{\omega\mathbf{k}}$ one can obtain in the first-order of $\tilde{G}$ the following expression for $\mathbf{E}^{rad}_{\omega\mathbf{k}}$

$$E^{rad}_{\omega\mathbf{k}} = \frac{i\omega^3 e}{2\pi^2}\frac{1}{k^2 - \omega^2\varepsilon}\int \frac{d^3k'}{k'^2 - \omega^2\varepsilon}\tilde{G}(\mathbf{k}' - \mathbf{k}) \times \left(\mathbf{V} - \frac{\mathbf{k}'}{\omega\varepsilon} - \mathbf{k}\frac{\mathbf{k}\cdot\mathbf{V} - \frac{\mathbf{k}\cdot\mathbf{k}'}{\omega\varepsilon}}{\omega^2\varepsilon}\right)\delta(\omega - \mathbf{k}'\cdot\mathbf{V}). \tag{4}$$

Formula for the spectral–angular distribution of the number of emitted photons follows from (4) in the form

$$\omega\frac{dN}{d\omega\, d\Omega} = e^2\omega^6 \int \frac{d^3k_1}{k_1^2 + 2\omega\sqrt{\varepsilon}\mathbf{n}\mathbf{k}_1}\frac{d^3k_2}{k_2^2 + 2\omega\sqrt{\varepsilon}\,\mathbf{n}\mathbf{k}_2}\langle\tilde{G}(\mathbf{k}_1)\tilde{G}^*(\mathbf{k}_2)\rangle \times \left[\left(\mathbf{V} - \frac{\mathbf{k}_1}{\omega\varepsilon}\right)\left(\mathbf{V} - \frac{\mathbf{k}_2}{\omega\varepsilon}\right) - \left(\mathbf{n}\mathbf{V} - \frac{\mathbf{n}\mathbf{k}_1}{\omega\varepsilon}\right)\left(\mathbf{n}\mathbf{V} - \frac{\mathbf{n}\mathbf{k}_2}{\omega\varepsilon}\right)\right] \times \delta\big(\omega(1 - \sqrt{\varepsilon}\,\mathbf{n}\mathbf{V}) - \mathbf{k}_1\mathbf{V}\big)\delta\big(\omega(1 - \sqrt{\varepsilon}\,\mathbf{n}\mathbf{V}) - \mathbf{k}_2\mathbf{V}\big), \tag{5}$$

where all interatomic correlations of interest to us are contained in the correlator $\langle\tilde{G}(\mathbf{k}_1)\tilde{G}^*(\mathbf{k}_2)\rangle$.

3. To show the possibility to use PB for study of short-range order in solids one should calculate above correlator using two-particle density $f_2(\mathbf{r}_l, \mathbf{r}_m)$ which may be presented as a sum $f_2(\mathbf{r}_l, \mathbf{r}_m) = f_1(r_l)f_1(r_m) + g_2(|\mathbf{r}_l - \mathbf{r}_m|)$, where $f_1 = 1/V$ is one-particle distribution function for a homogeneous target, V is the volume of this target, g_2 is the two-particle correlation function. The desired radial density is expressed in term of the correlation function by the formula $n_0 V^2 n(r) = n(r) - n_0$ [6]. Based on above considerations one can represent (5) in the form

$$\omega\frac{dN}{d\omega\, d\Omega} = \omega\frac{dN_0}{d\omega\, d\Omega} + \omega\frac{d\Delta N}{d\omega\, d\Omega}, \tag{6}$$

where the first item in the right side describes PB generated independently on each atom of the target

$$\omega\frac{dN_0}{d\omega\, d\Omega} \simeq \frac{2Z^2e^6}{\pi m^2}Ln_0\left|\frac{\omega^2}{\omega_p^2}\chi(\omega)\right|^2 \times \frac{1}{(1 + 4\omega^2R^2)^2}\left(\ln\sqrt{\frac{1 + 4\omega^2R^2}{\omega^2R\rho^2}} - 1\right). \tag{7}$$

Here Z is the number of electrons in a target atom, L is the thickness of the target, ω_p is the plasma frequency, $\rho^2 = \gamma^{-2} + \omega_p^2/\omega^2$, γ is Lorentz factor of an emitting fast electron.

The last item in (6) describes an addition to PB caused by interatomic correlations

$$\omega\frac{d\Delta N}{d\omega\, d\Omega} = \frac{4Z^2e^6}{m^2\omega}Ln_0\left|\frac{\omega^2}{\omega_p^2}\chi(\omega)\right|^2 \times \int_1^\infty \frac{dx}{(1 + 4\omega^2R^2x^2)^2}\frac{x^2 - 1}{(x^2 - 1 + \frac{1}{4}\rho^2)^2} \times \int_0^\infty dr\, r\big(n(r) - n_0\big)\sin(2\omega r x). \tag{8}$$

Obviously the difference between the total PB spectral–angular distribution $\omega\frac{dN}{d\omega\, d\Omega}$ which may by measured experimentally and PB calculated within the frame of independent contribution of different atoms to PB yield $\omega\frac{dN_0}{d\omega\, d\Omega}$ allows one to determine conceptually the function $n(r)$.

It is important to keep in mind that the results (7) and (8) have been obtained to fit PB photons emitted in a backward direction relative to an emitting electron velocity. This is of no concern for PB on a separate atom (7). On the other hand, it is of fundamental importance in the task of $\omega\frac{d\Delta N}{d\omega\, d\Omega}$ determination on the base of the result (8). Indeed, the connection between Fourier transform of radial density $n(r)$ and the quantity $\omega\frac{d\Delta N}{d\omega\, d\Omega}$ is integral, but in conditions of PB in a backward direction under consideration this connection can be approximated by local one due to extremely small value of the width of the range of momentum transfer, as it follows immediately from the coefficient $(x^2 - 1)/(x^2 - 1 + \rho^2/4)^2$ consisting in a very sharp peak with the width of the order of $\rho^2/4 \approx 1/4\gamma^2 \ll 1$.

Since the effective values of r in the integral (8) is in the region of a distance between atoms l, the variable x in the function $\sin(2\omega r x)$ is approximately equal to unity with the proviso that

$$\frac{1}{4}\omega l\rho^2 \approx \frac{1}{4}\omega l\gamma^{-2} \ll 1. \tag{9}$$

As a result the formula (8) takes the form

$$\omega\frac{d\Delta N}{d\omega\, d\Omega} \approx A(\omega)\int_0^\infty dr\, r\big(n(r) - n_0\big)\sin(2\omega r),$$
$$A(\omega) = \frac{2Z^2e^6}{m^2\omega}Ln_0\left|\frac{\omega^2}{\omega_p^2}\chi(\omega)\right|^2\frac{1}{(1 + 4\omega^2R^2)^2}\ln\frac{16}{\rho^2}. \tag{10}$$

Obviously, quantities described by formulae (7) and (10) allow one to determine the desired radial density as

$$n(r) - n_0 = \frac{1}{r}\frac{4}{\pi}\int_0^\infty d\omega\sin(2\omega r)\frac{\omega\frac{dN}{d\omega\, d\Omega} - \omega\frac{dN_0}{d\omega\, d\Omega}}{A(\omega)}, \tag{11}$$

where PB spectral–angular distribution $\omega\frac{dN}{d\omega\, d\Omega}$ is defined from the experiment. It is of first importance that Eq. (11) does not involve distortions in the function $n(r)$ in distinction to analogous Zernicke–Prins equation [7]. This is due to EDXD approach and well defined spectrum of initial virtual photons.

4. Formula (11) tackles the problem being considered conceptually. Let us estimate the necessary conditions for realization of proposed method in experiment.

Since the angular spread of PB is of about γ^{-1}, initial angular spread of emitting electron beam ψ_0 and multiple scattering angle achievable at the target length $\psi_S = \sqrt{\frac{\varepsilon_k^2 L}{m^2\gamma^2 L_R}}$ must be less then γ^{-1}, here $\varepsilon_k \approx 20$ MeV, L_R is radiation length. Furthermore, the addition to PB (10) must exceed background from the side of ordinary bremsstrahlung and transition radiation emitted to backward direction. Reasoning for simplicity $n(r) \approx n_0\sigma(r - l)$ and calculating

integral (10) and bremsstrahlung yield one can derive the condition for neglecting of bremsstrahlung in the form

$$\ln\left(\frac{4}{\rho^2}\right)\frac{F(2\omega l)}{(1+4\omega^2R^2)^2} \gg \frac{1}{2\pi\gamma^2}\ln\frac{mR}{\sqrt{1+4\omega^2R^2}}, \tag{12}$$

where $F(x)=\frac{3}{8x^3}(\sin x - x\cos x)$. Obviously, this condition can be fulfilled in a wide region of task parameters. Analogous condition for neglecting of transition radiation

$$\ln\left(\frac{4}{\rho^2}\right)\frac{F(2\omega l)}{(1+4\omega^2R^2)^2} \gg \frac{\gamma^2}{\omega^4 l^4}\frac{l}{L} \tag{13}$$

is easily executable as well.

5. Conclusions

The performed analysis opens the way to create a new EDXD method of the diagnostics of radial density for atoms in a dense medium on the base of relativistic electron PB in a backward direction.

The desired function is reconstructed by Eq. (11). The field of integration in this equation is not bounded from overhead, which is why the desired function is not distorted in distinction to Zernicke–Prins approach.

Employment of electron PB allows one to develop the method of structure diagnostics with high space resolution by focusing of a primary electron beam on the sample using magnetic optics.

Proposed method can be realized by the use of electron beams with relatively small energies of about 10 MeV.

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