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X-ray surface back diffraction

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A new case of X-ray surface back diffraction (SBD), combining features of surface diffraction (grazing of the beams along a crystal surface) and back diffraction (Bragg angle is close to 90°) is studied, both theoretically and experimentally. Dynamical diffraction theory is given for two- and four-wave SBD. Experimental measurements of transmitted and back diffracted intensities are carried out for four-wave SBD of Co $K_{\alpha 1}$ radiation from (620) planes of a Ge crystal. It is shown that a number of effects inherent to SBD – a large angular width of reflections, an extreme sensitivity of rocking curves for lattice spacing in a crystal surface layer, the existence of a narrow multiwave dip and the variation of the exit angle of back diffracted waves on rocking curves – may prove to be very useful in synchrotron radiation optics and surface studies with synchrotron radiation.

1. Introduction

Recently, researchers have shown an increased interest in extreme cases of X-ray diffraction, such as surface diffraction under conditions of total external reflection [1–4] and back diffraction with Bragg angle close to 90° [5–8]. In the first scheme, owing to the grazing geometry of diffraction and the effect of total reflection, a diffracted wave is formed in a thin surface layer of a crystal ~ 10–100 Å in depth only, that permits one to study the crystal surface. In the second scheme the extreme scattering angle provides maximum sensitivity of diffraction curves to a change of the wavelength and of the lattice parameter in a crystal. Besides, at back diffraction a strong (by two to three orders of magnitude) broadening of the angular diffraction region compared to the width of standard Bragg peaks is observed. The given properties of this scheme are proposed to be used respectively for absolute measurement of the lattice parameter of crystals (extreme Bond method [8]), for the analysis of inelastic scattering [9–11] and for intensive X-ray focusing [12].

Subject of research in the present report is the diffraction scheme, combining the conditions of a surface diffraction (grazing of beams along a crystal surface) with the back diffraction condition ($\theta_B \approx 90°$), which we call the surface back diffraction (SBD).

To realize SBD, two conditions have to be simultaneously satisfied:

1) Diffraction planes are normal to the crystal surface or misoriented from the surface normal by an angle φ, not exceeding in order of magnitude the critical angle ϕ_c of total external X-ray reflection: $\phi_c \equiv \sqrt{|\chi_0|} \leq 10^{-3}$–$10^{-2}$ rad (χ_0 is the zeroth Fourier component of crystal polarizability).

2) The radiation wavelength λ is equal to a double interplanar spacing d, or to be more exact, the following condition is satisfied [6]:

$$2d(1-\epsilon) = \lambda, \tag{1}$$

where $|\epsilon| \leq |\chi_0| \approx 10^{-5}$–$10^{-6}$ is the parameter replacing the Bragg angle, as the latter one under conditions of back diffraction not always has a physical meaning ($\theta_B = \pi/2 - \sqrt{2\epsilon}$, and for $\lambda > 2d$ parameter ϵ becomes negative and hence θ_B complex).

The SBD scheme was earlier proposed in ref. [13]. In ref. [14] a specific case of coplanar SBD was theoretically analyzed. In refs. [15,16] we published the first results of experimental SBD studies.

In the given work, a full systematic study of SBD effects on the basis of the two- and four-wave dynamical diffraction theory is presented. Experimental verification of the theory on a transmitted and a diffracted beam for SBD of Co $K_{\alpha 1}$ radiation from planes (620) of a germanium crystal is carried out.

2. Two-wave SBD theory

The simplest way of building the two-wave SBD theory consists in the use of the results of ref. [6] and refs. [1,3,4]. It was shown in ref. [6] that in passing from

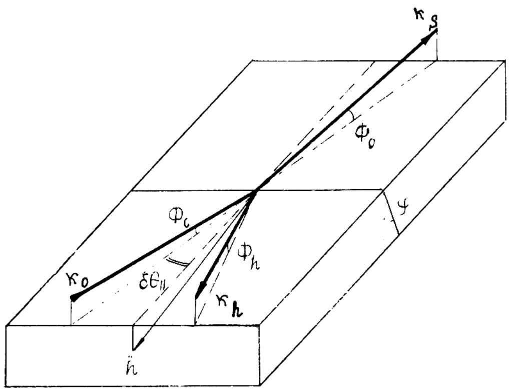

Fig. 1. Surface back diffraction layout. $\boldsymbol{\kappa}_0$, $\boldsymbol{\kappa}_h$, $\boldsymbol{\kappa}_s$ are the wave vectors of incident, back diffracted and specularly reflected waves, respectively, $\boldsymbol{h}$ is the reciprocal lattice vector, ϕ_0 is the angle of incidence, ϕ_h is the exit angle of a back diffracted wave, $\delta\theta_{\|}$ is the angle between the projections of vectors $\boldsymbol{\kappa}_0$ and $\boldsymbol{h}$ on the crystal surface.

scattering with standard Bragg angles to back diffraction ($\theta_B \to 90°$), the form of diffraction equations is preserved; only the angular dependence of α changes in this. Here α is a standard parameter, characterizing the deviation of an incident X-ray wave from the Bragg condition:

$$\alpha = \frac{2\boldsymbol{\kappa}_0\boldsymbol{h} + \boldsymbol{h}^2}{\boldsymbol{\kappa}_0^2}, \tag{2}$$

where $\boldsymbol{\kappa}_0$ is the wave vector of an incident wave, $\boldsymbol{h}$ is the reciprocal lattice vector. That is why in case of two-wave SBD we can apply formulas for describing the surface diffraction from refs. [1,3,4] in which the dependence of α is replaced.

To determine the angular dependence of α we shall consider the SBD scheme, presented in fig. 1. An incident wave makes small angles ϕ_0 and $\delta\theta$ with the crystal surface and vector $\boldsymbol{h}$. Here the back diffraction condition (1) is fulfilled, it may be rewritten in the form

$$2\kappa_0(1-\epsilon) = h. \tag{3}$$

From eqs. (2) and (3) follows the angular dependence of α in the form

$$\alpha = 2(\delta\theta^2 - 2\epsilon). \tag{4}$$

It is convenient to decompose the angular deviation $\delta\theta$ into two mutually perpendicular components, measured along the surface and along the surface normal: $\delta\theta^2 = \delta\theta_{\|}^2 + (\phi_0 + \varphi)^2$. Here $\delta\theta_{\|}$ is the angle between the projections of $\boldsymbol{\kappa}_0$ and $\boldsymbol{h}$ at the crystal surface. Finally we obtain

$$\alpha = 2\left[\delta\theta_{\|}^2 + (\phi_0 + \varphi)^2 - 2\epsilon\right]. \tag{5}$$

Eq. (5) permits one to characterize at once a number of SBD properties. Firstly, not only changes of $\delta\theta_{\|}$, but also those of ϕ_0 contribute to changes of α. In other words, ϕ_0 becomes a diffraction angle, whereas in a usual surface diffraction scheme ($\pi/2 - \theta_B \sim 1$ rad) the parameter α depends practically on one angle $\theta \equiv \pi/2 - \delta\theta$ alone and ϕ_0 may be chosen arbitrary. Secondly, since diffraction takes place at values $|\alpha| \le |\chi_0|$, the width of Bragg maxima, in case of scanning both in ϕ_0 and in $\delta\theta_{\|}$, is of the order of $\sqrt{|\chi_0|} \sim 10^{-2}$–$10^{-3}$ rad. Thus, owing to the quadratic dependence of α on the angles in eq. (5), the width of diffraction SBD maxima will be by two to three orders greater than usually and will constitute dozens of minutes of arc. Large angular width of SBD maxima was mentioned earlier in ref. [13]. Thirdly, when scanning in $\delta\theta_{\|}$, an incident beam intersects twice the exact Bragg position $\alpha = 0$ at points $\delta\theta_{\|} = \pm[2\epsilon - (\phi_0 + \varphi)^2]^{1/2}$. At sufficiently large values of $\epsilon > |\chi_0|$ two respective Bragg peaks will appear separately, and $\epsilon(d)$ may be determined from the distance between them. Thus SBD may serve as a basis for the realization of a very sensitive Bond method for thin surface layers of crystals. The thickness of these layers is determined by a radiation penetration into a crystal in case of surface diffraction and constitutes ~ 10–100 Å.

Nonstandard angular dependence, eq. (5), of the parameter α determines one more property of SBD, connected with exit angles of back diffracted waves. To estimate the magnitude of the exit angles ϕ_h we shall use the relation between ϕ_h, ϕ_0 and α, set up in ref. [4] as applied to the general case of a surface diffraction:

$$\phi_h^2 = (\phi_0 + \psi)^2 - \alpha. \tag{6}$$

Here ψ is the effective angle of diffraction planes misorientation with respect to the surface normal (for SBD $\psi \approx 2\varphi$). Substituting eq. (5) into eq. (6), we obtain

$$\phi_h^2 = \phi_I^2 - \phi_0^2 - 2\,\delta\theta_{\|}^2, \tag{7}$$

where $\phi_I^2 \equiv 2(\varphi^2 + 2\epsilon)$ is the critical angle of total internal reflection of back diffracted waves.

As follows from eq. (7), the exit angle of a back diffracted wave cannot exceed ϕ_I. As any of the diffraction angles ϕ_0 or $|\delta\theta_{\|}|$ increases, angle ϕ_h diminishes and becomes an imaginary one. The intensity of a back diffracted beam in vacuum sharply decreases in this case, which corresponds to total internal reflection. As a diverging monochromatic X-ray beam is incident on a crystal, back diffracted beam forms a semicone: $\phi_h \ge 0$ and $\phi_h^2 + 2\,\delta\theta_{\|}^2 \le \phi_I^2$. Thus, SBD has the property of a tail-less collimation of monochromatic X-ray radiation (for example, Mössbauer one) in two planes.

Substitution of eqs. (5) and (7) into reflection and transmission coefficients for a surface diffraction, found in ref. [4], solves entirely the problem of theoretically describing the two-wave SBD. It should be noted that,

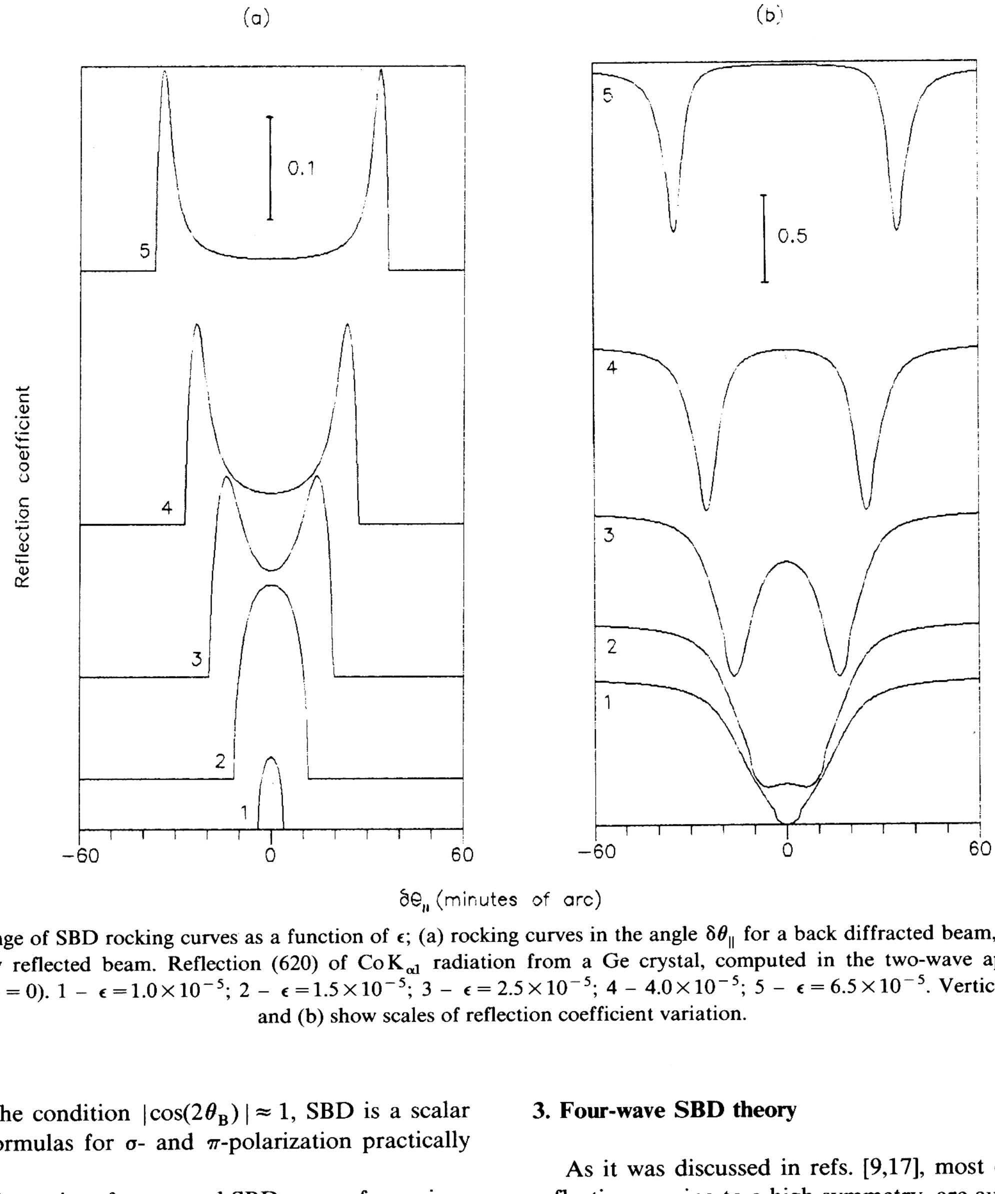

Fig. 2. Change of SBD rocking curves as a function of ϵ; (a) rocking curves in the angle $\delta\theta_{\parallel}$ for a back diffracted beam, (b) those for a specularly reflected beam. Reflection (620) of $\mathrm{Co\,K_{\alpha 1}}$ radiation from a Ge crystal, computed in the two-wave approximation ($\phi_0 = 21'$, $\varphi = 0$). 1 – $\epsilon = 1.0 \times 10^{-5}$; 2 – $\epsilon = 1.5 \times 10^{-5}$; 3 – $\epsilon = 2.5 \times 10^{-5}$; 4 – 4.0×10^{-5}; 5 – $\epsilon = 6.5 \times 10^{-5}$. Vertical lines in (a) and (b) show scales of reflection coefficient variation.

owing to the condition $|\cos(2\theta_B)| \approx 1$, SBD is a scalar one, i.e. formulas for σ- and π-polarization practically coincide.

In fig. 2 a series of computed SBD curves for various ϵ depending on $\delta\theta_{\parallel}$ is presented. Computations were made for SBD of $\mathrm{Co\,K_{\alpha 1}}$ radiation from planes (620) of a Ge crystal at an angle of incidence $\phi_0 = 21'$. Fig. 2a shows reflection coefficients for back diffracted waves, fig. 2b shows the same for transmitted (specularly reflected) waves. The figure clearly demonstrates the high potential of SBD in measuring the crystal lattice parameter, because small changes of $\Delta\epsilon = \Delta d/d \sim 10^{-5}$ in an explicit form manifest themselves over the range of minutes of arc on the diffraction curve pattern. It should be noted that a possibility to carry out measurements on a transmitted beam considerably simplifies the realization of the method, as the main experimental difficulties are related with the detection of a back diffracted beam.

3. Four-wave SBD theory

As it was discussed in refs. [9,17], most of the back reflections, owing to a high symmetry, are automatically accompanied by additional reflections, i.e. they have a multiwave character. In fact, since the vector $\boldsymbol{h}_1$, corresponding to a back diffraction, is the diameter of the Ewald sphere, any two vectors $\boldsymbol{h}_2$ and $\boldsymbol{h}_3$, satisfying the conditions

$$\boldsymbol{h}_2 \perp \boldsymbol{h}_3 \quad \text{and} \quad \boldsymbol{h}_2 + \boldsymbol{h}_3 = \boldsymbol{h}_1, \tag{8}$$

automatically find themselves in a Bragg state. If the number of vector pairs, satisfying conditions (8) is equal to N, then SBD will lead to a $(2N+2)$-wave. For example, SBD on planes (620) in Ge treated in the previous section in a two-wave approximation is a four-wave SBD with the excitation of additional (440) and $(2\bar{2}0)$ reflections.

Let us analyze a four-wave SBD in the case where additional vectors $\boldsymbol{h}_2$ and $\boldsymbol{h}_3$ are parallel to the crystal surface, i.e. they satisfy the conditions of surface diffraction. This case is a typical one as concerns the occurrence of multiwave effects. It is experimentally realized in measuring SBD from (620) planes in Ge with the (001) surface orientation.

To determine the intensity of all diffracted waves and of the transmitted (specularly reflected) one, it is necessary to find the dependence of parameters α_2 and α_3 on diffraction angles ϕ_0 and $\delta\theta_{\|}$ and to solve the set of equations, consisting of diffraction equations in a crystal and boundary conditions for tangential field components and their derivatives at a crystal surface.

We can find α_2 and α_3 by decomposing the wave vector of an incident wave, $\boldsymbol{\kappa}_0$, into projections along vectors $\boldsymbol{n}$ (the unity vector perpendicular to the crystal surface), $\boldsymbol{h}_1$ and $[\boldsymbol{n} \times \boldsymbol{h}_1]$, and then substituting the decomposition in definitions of α_2, α_3 of the form of eq. (2):

$$\alpha_2 = -2\,\delta\theta_{\|}\,\sin(2\theta_{B2}) + 4\varphi_2(\phi_0 + \varphi_1)\,\sin(\theta_{B2}) - 2\left(2\epsilon + \varphi_1^2 - \phi_0^2\right)\,\sin^2(\theta_{B2}), \tag{9}$$

$$\alpha_3 = 2\,\delta\theta_{\|}\,\sin(2\theta_{B3}) + 4\varphi_3(\phi_0 + \varphi_1)\,\sin(\theta_{B3}) - 2\left(2\epsilon + \varphi_1^2 - \phi_0^2\right)\,\sin^2(\theta_{B3}). \tag{10}$$

Here φ_1, φ_2, φ_3 are the small angles of misorientation of $\boldsymbol{h}_1$, $\boldsymbol{h}_2$, $\boldsymbol{h}_3$ with respect to the crystal surface ($\varphi_l > 0$ for the misorientation in the direction of an internal normal).

From eqs. (9) and (10) immediately follows that, owing to a linear dependence of α_2 and α_3 on $\delta\theta_{\|}$, multiwave effects on SBD curves occurs within a very narrow region about the centre: $|\delta\theta_{\|}| \le |\epsilon|/\sin(2\theta_{B2}) \sim 10^{-5}$–$10^{-6}$ rad. The distance between two multiwave points $\alpha_2 = 0$ and $\alpha_3 = 0$ within this region is proportional to $|\epsilon|/\sin(2\theta_{B2})$, so at $|\epsilon| \ge |\chi_0|$ two narrow multiwave dips will be resolved in the SBD curves, and at $|\epsilon| < |\chi_0|$ only one.

Passing to evaluation of reflection coefficients, for simplicity we shall confine ourselves to waves polarized perpendicularly to the surface (σ-polarization). Neglecting a small noncoplanarity of the scattering layout, the diffraction equations in a crystal may be written in the form (cf. ref. [4])

$$\mathbf{S} \times \boldsymbol{D} = 0, \tag{11}$$

$$\mathbf{S} = \begin{bmatrix} u^2 - \phi_0^2 - \chi_0 & -\chi_{01} & -\chi_{02} & -\chi_{03} \\ -\chi_{10} & (u+\psi_1)^2 - \phi_1^2 - \chi_0 & -\chi_{12} & -\chi_{13} \\ -\chi_{20} & -\chi_{21} & (u+\psi_2)^2 - \phi_2 - \chi_0 & -\chi_{23} \\ -\chi_{30} & -\chi_{31} & -\chi_{32} & (u+\psi_3)^2 - \phi_3^2 - \chi_0 \end{bmatrix}$$

is the scattering matrix, χ_{hl} are the crystal polarizabilities, ψ_1, ψ_2, ψ_3 are the effective angles of diffraction plane misorientation ($\psi_1 = 2\varphi_1$, $\psi_2 = 2\varphi_2\sin(\theta_{B2})$, $\psi_3 = 2\varphi_3\sin(\theta_{B3})$), ϕ_1, ϕ_2, ϕ_3 are the exit angles of diffracted waves from a crystal, related with the corresponding α from eqs. (5), (9) and (10) by equations of the form of eq. (6), $\boldsymbol{D} = (D_0, D_1, D_2, D_3)$ is the vector composed of the amplitudes of the incident and diffracted waves in a crystal.

The compatibility condition for eqs. (11) – the dispersion equation – assumes the form

$$\det\{\mathbf{S}(u)\} = 0. \tag{12}$$

Since this equation is a polynomial of degree 8 in u, it has eight solutions of $u^{(j)}$. Four solutions with $\mathrm{Im}(u^{(j)}) > 0$ conform to the wave attenuation into the crystal depth, and four solutions with $\mathrm{Im}(u^{(j)}) < 0$ conform to the increase in wave amplitudes. For a thick crystal four attenuating modes of $\boldsymbol{D}^{(j)}$ with $\mathrm{Im}(u^{(j)}) > 0$ should be chosen. On evaluation of the roots of eq. (12), the set of eqs. (11) allows one to express the amplitudes of waves D_1, D_2, D_3 in terms of D_0:

$$D_l^{(j)} = C_l^{(j)} D_0^{(j)}, \quad l = 1, 2, 3. \tag{13}$$

Boundary conditions at the crystal surface take the form

$$E_0 + E_s = \sum_{j=1}^{4} D_0^{(j)}, \quad \phi_0(E_0 - E_s) = \sum_{j=1}^{4} u^{(j)} D_0^{(j)}, \tag{14a}$$

$$E_l = \sum_{j=1}^{4} D_l^{(j)}, \quad -\phi_l E_l = \sum_{j=1}^{4} \left(u^{(j)} + \psi_l\right) D_l^{(j)}, \tag{14b}$$

for $l = 1, 2, 3$. Here E_0, E_s, E_1, E_2, E_3 are amplitudes of the incident, specularly reflected and diffracted waves in vacuum in front of the crystal surface.

After substituting eq. (13) into eq. (14), we obtain a set consisting of eight equations with respect to eight unknown amplitudes of the fields E_s, E_1, E_2, E_3, $D_0^{(1)}$, $D_0^{(2)}$, $D_0^{(3)}$, $D_0^{(4)}$. This set of equations is easily solved by a Gaussian method. On finding the wave amplitudes, reflection coefficients are evaluated according to the formulas ($l = 1, 2, 3$)

$$P_0 = |E_s/E_0|^2, \quad P_l = \frac{\mathrm{Re}\phi_l}{\phi_0}|E_l/E_0|^2. \tag{15}$$

The analysis made is simply generalized for the π-polarization case, and, hence it solves completely the problem of describing a four-wave SBD.

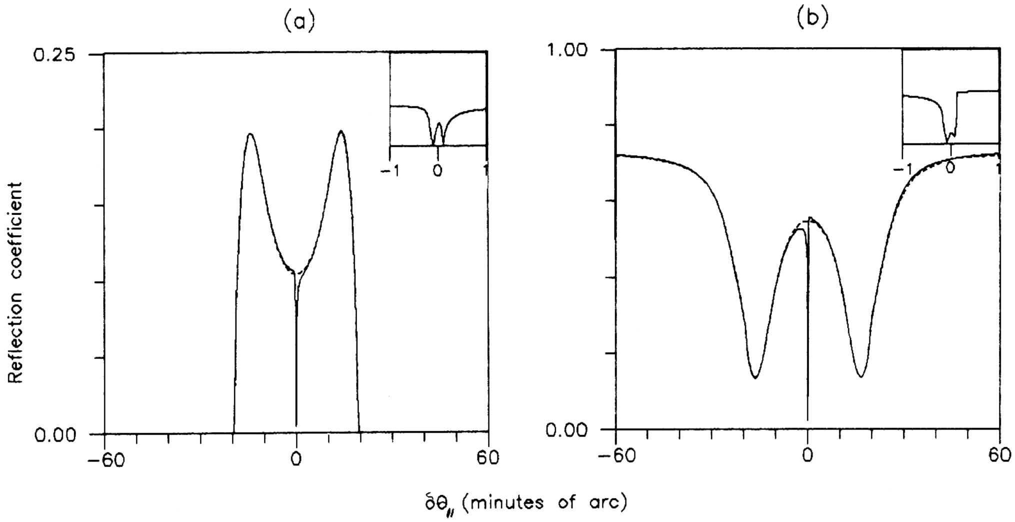

Fig. 3. Comparison of SBD curves, computed in the two-wave (dashed line) and four-wave (full line) approximation; (a) rocking curves in the angle $\delta\theta_{\parallel}$ for a back diffracted beam, (b) those for a specularly reflected beam. A fine structure of the four-wave diffraction region (620), ($2\bar{2}0$), (440) is shown in the inserts. Computation parameters are the same as in fig. 2, $\epsilon = 2.5 \times 10^{-5}$.

SBD rocking curves of Co $K_{\alpha 1}$ radiation from planes (620) of a Ge crystal, computed in the two-wave and four-wave approximation for $\epsilon = 2.5 \times 10^{-5}$ and $\phi_0 = 21'$, are compared in fig. 3. It is well seen that with the exception of a narrow central region the two-wave approximation is quite adequate, which allows a considerable simplification of the computations. On the other hand, the narrow multiwave dip may serve as a precise origin for an angular matching of SBD curves. A fine structure of this dip, showing the separation of ($2\bar{2}0$) and (440) reflections is presented on the inserts.

4. Experimental

To realize SBD experimentally, we need:

- to provide the angular collimation of an incident beam in two planes with an accuracy not worse than ~ 1 minute of arc.
- to determine a fixed radiation wavelength satisfying the back diffraction condition $\lambda = 2d$ with an accuracy up to $\Delta\lambda/\lambda < 10^{-5}$.
- to provide the beam front along the normal to the surface not worse than ≤ 50 μm in view of small angles of incidence.
- to solve the problem of detection of a back diffracted beam, i.e. to separate it from an incident one.

These problems were partially solved in refs. [4,18–20] and in refs. [7,8]; in these works measurements of surface diffraction and back diffraction in the Bragg geometry were respectively carried out. The back diffraction condition $\lambda = 2d$ is simply satisfied with synchrotron radiation. For characteristic X-rays there are few combinations of X-ray lines and diffracting planes, found in ref. [5].

We made an experimental study of SBD effects for the first time. Reflection of Co $K_{\alpha 1}$ radiation from (620) planes of a Ge crystal with the (001) surface orientation was used. The misorientation of the surface from (001) did not exceed $|\varphi| \leq 0.5'$.

The experimental layout is presented in fig. 4. An X-ray beam from the 1.3 kW source (1) with focus 400×800 μm^2 was collimated in the horizontal plane (with respect to $\delta\theta_{\parallel}$) accurate up to $\sim 0.1'$ by means of

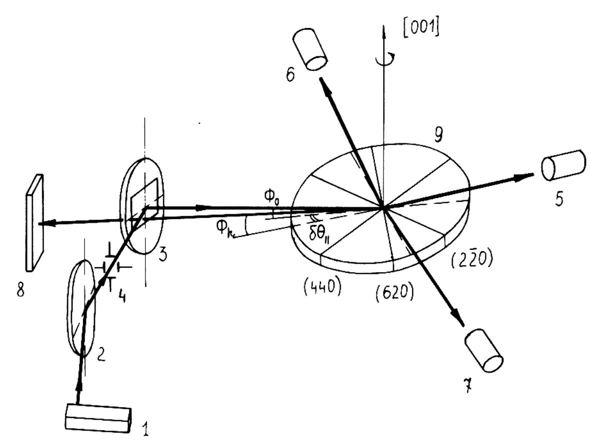

Fig. 4. Schematic illustration of the experiment. 1 – X-ray tube, 2 – the first monochromator, 3 – the second monochromator with a semitransparent window, 4 – slits, 5, 6, 7 – scintillation detectors, 8 – position sensitive detector, 9 – sample.

two Si monochromators (2) and (3) (reflections (220) and (400)). Collimation in the vertical plane (with respect to the incidence angle ϕ_0) accurate within $\sim 1'$ was performed by slit (4), 20 μm in width. Owing to the nonparallel arrangement of the monochromators and the presence of slit (4), the collimating system cuts the radiation with a fixed wavelength with an accuracy up to $\Delta\lambda/\lambda \leq 3 \times 10^{-5}$. Turning of the crystal (2) permitted to vary λ within the Co $K_{\alpha 1}$ line. The specularly reflected beam was counted by detector (5), and additional diffraction beams ($2\bar{2}0$) and (440) by detectors (6) and (7), respectively. For detecting the back diffracted beam a semitransparent window with dimensions 1.5×1.5 cm^2 and ~ 15 μm thick was etched in

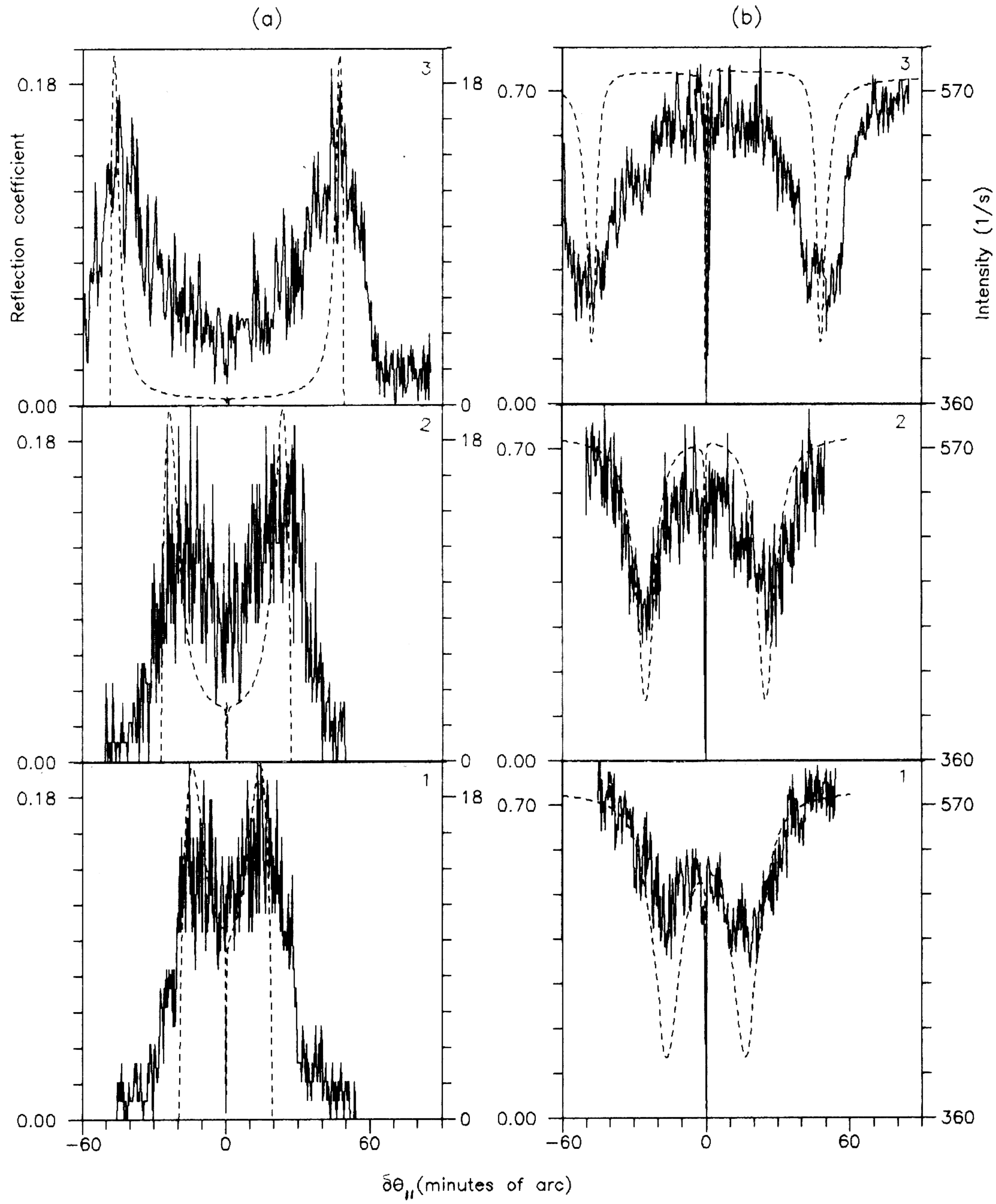

Fig. 5. Comparison of experimental and theoretical SBD curves; (a) rocking curves in the angle $\delta\theta_{\parallel}$ for a back diffracted beam, (b) those for a specularly reflected beam. Full lines show experimental curves, dashed lines those computed in the four-wave approximation, for: 1 – $\epsilon = 2.5 \times 10^{-5}$; 2 – $\epsilon = 4.0 \times 10^{-5}$; 3 – $\epsilon = 11.0 \times 10^{-5}$. The remaining computation parameters are the same as in figs. 2 and 3.

the crystal monochromator (3). The incident beam was Bragg reflected from the window surface, and the back diffracted one passed through the window with an approximately two-fold attenuation, apart from a very narrow region of strict back diffraction $|\delta\theta_{\|}| \leq 5''$ in which this beam also satisfied the Bragg condition for crystal monochromator (3). After passing through monochromator (3) the back diffracted beam was detected by a vertically arranged position sensitive detector (PSD) (8). Application of a PSD enabled us to separate with respect to the magnitude of an exit angle a surface back diffracted beam of interest from the beam which back diffracted in the Bragg geometry from the lateral face of a sample, because the difference of exit angles of the beams was equal to $\phi_h + \phi_0$. The angle of incidence of $\phi_0 = 21'$ was chosen in the experiment and the beams diverged on the PSD rule by 2–4 mm.

Adjustment of sample (9) was carried out with the aid of additional reflections $(2\bar{2}0)$ and (440). Fulfilment of the back diffraction condition $|\epsilon| \leq 10^{-5}$ was achieved through the variation of the sample temperature, which was checked by the coincidence of the angular positions of $(2\bar{2}0)$ and (440) peaks. Coincidence was reached at $t = 17\,°C$. Then the radiation wavelength was varied within the Co $K_{\alpha 1}$ line to specify different ϵ, and rocking curves of SBD depending on $\delta\theta_{\|}$ were recorded.

5. Results and discussion

Results are given in fig. 5. The dashed lines in the same figure show corresponding theoretical curves for a perfect crystal, computed based on the four-wave theory without account of experimental spreading. Computation parameters were $\phi_0 = 21'$, $\varphi_1 = \varphi_2 = \varphi_3 = 0$, $\epsilon = 2.5 \times 10^{-5}$, 4×10^{-5} and 11×10^{-5}. The parameter ϵ, used in computations, was estimated from experiment according to the angular distance between the dips on rocking curves of the specularly reflected beam (fig. 5b). Angular matching of theory with experiment was carried out according to the superposition of a multiwave dip on curves of the specularly reflected beam. When matching specular reflection curves according to the intensity scale, the tails and minimum of a multiwave dip were brought into coincidence. Large background of ~ 360 pulses/s on experimental curves at fig. 5b is attributed to the fact that a portion of the incident beam strikes the counter (5) in passing by the sample.

The fine structure of the multiwave region was not resolved in the present experiment for $\epsilon \leq 11 \times 10^{-5}$. Therefore, inserts analogous to that in fig. 3 are not shown in fig. 5.

A qualitative agreement of theory with experiment is observed. For a more exact comparison, theoretical curves should be averaged within the experimental resolution $\Delta\epsilon = 3 \times 10^{-5}$, and the presence of an amorphous layer on a crystal surface should be taken into account. But evaluations show that this is not sufficient and a noticeable broadening of experimental curves in comparison with theoretical ones should be attributed to the interplanar distance spread in a surface layer of the crystal.

Thus, when using synchrotron radiation or any other X-ray radiation with a white spectrum, the SBD method may be applied for the precise determination of a lattice parameter on a crystal surface. Accuracy of this method is $\Delta d/d \leq 10^{-6}$, which is an order of magnitude higher than the accuracy provided by the surface Bond method, presented in ref. [21]. In fact, in our experiment the method of ref. [21] served for a preliminary multiwave SBD adjustment. We should note that to realized the Bond method on the SBD basis there is no need in a semitransparent window and PSD, as all the measurements can be made on a transmitted (specularly reflected) beam.

Diffraction curves of a back diffracted beam in fig. 5a are characterized by sharp decreases in intensity on tails down to background oscillations level. We think that these sharp decreases are due to the decrease of the exit angle and to the total internal reflection of back diffracted waves. The decrease of the exit angle of back diffracted waves in case of an increase in $|\delta\theta_{\|}|$ was also detected with the help of PSD.

Concluding, experiments confirmed the SBD properties predicted – a large angular width, the presence of two maxima with the distance between them depending on λ/d, the existence of a narrow multiwave dip and the variation of the exit angle of back diffracted waves on rocking curves. We believe, that the discussed effects may prove to be very useful for application in synchrotron radiation optics and surface studies with synchrotron radiation.

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References

[1] V.G. Baryshevskii, Sov. Tech. Phys. Lett. 2 (1976) 43.
[2] W.C. Marra, P. Eisenberger and A.Y. Cho, J. Appl. Phys. 50 (1979) 6927.
[3] A.M. Afanas'ev and M.K. Melkonyan, Acta Crystallogr. A39 (1983) 207.
[4] P.A. Aleksandrov, A.M. Afanas'ev, A.L. Golovin, R.M.

Imamov, D.V. Novikov and S.A. Stepanov, J. Appl. Crystallogr. 18 (1985) 27.
[5] K. Kohra and T. Matsushita, Z. Naturforsch. A27 (1972) 484.
[6] S. Caticha and S. Caticha-Ellis, Phys. Rev. B25 (1982) 971.
[7] V.I. Kushnir and E.V. Suvorov, JETP Lett. 44 (1986) 262.
[8] Yu. P. Stetsko, S.A. Kshevetskii and I.P. Mikhailyuk, Sov. Tech. Phys. Lett. 14 (1988) 13.
[9] W. Graeff and G. Materlik, Nucl. Instr. and Meth. 195 (1982) 97.
[10] B. Dorner and J. Peisl, Nucl. Instr. and Meth. 208 (1983) 587.
[11] B. Dorner, E. Burkel and J. Peisl, Nucl. Instr. and Meth. A246 (1986) 450.
[12] V.I. Kushnir and E.V. Suvorov, JETP Lett. 48 (1988) 117.
[13] S.A. Maksimenko, Phys. Stat. Sol. A85 (1984) K23.
[14] A.P. Bezirganyan and P.A. Bezirganyan, Phys. Stat. Sol. A105 (1988) 345.
[15] S.A. Stepanov, E.A. Kondrashkina and D.V. Novikov, Collected Abstr. XII Europ. Crystallogr. Meeting, vol. 2 (Moscow, 1989) p. 104.
[16] D.V. Novikov, E.A. Kondrashkina and S.A. Stepanov, Phys. Stat. Sol. A114 (1989) K7.
[17] R. Collela and A. Luccio, Optics Commun. 50 (1984) 41.
[18] A.L. Golovin, R.M. Imamov and S.A. Stepanov, Acta Crystallogr. A40 (1984) 225.
[19] A.L. Golovin, R.M. Imamov and E.A. Kondrashkina, Phys. Stat. Sol. A88 (1985) 505.
[20] P.L. Cowan, S. Brennan, T. Jack, M.J. Bedzik and G. Materlik, Phys. Rev. Lett. 57 (1986) 2399.
[21] A.L. Golovin, R.M. Imamov and E.A. Kondrashkina, Phys. Stat. Sol. A89 (1985) K5.