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## **X-Ray Standing Waves under the Conditions of Multiple Diffraction**

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Equations are obtained for calculating the angular dependence of the secondary radiation yield (the photoelectron emission or fluorescence radiation) under the conditions of multiple dynamical X-ray diffraction. For a small yield depth  $L_{yi}$  the intensity of secondary radiation is proportional to the intensity of X-rays at the atomic sites of a surface layer of the single crystal. If  $L_{yi} > L_A$ , where  $L_A$  is the X-ray penetration depth, then the secondary radiation intensity is proportional to the total absorbed energy of X-rays. Computer simulation of the threewave case (444, 335, Bragg geometry,  $\text{CuK}_\alpha$ , Si) shows that the angular dependence of the photoelectron emission yield can be described as a repulsion interaction of two crossing two-wave maxima. New possibility of observing the two-wave X-ray standing waves is discussed where the angular dependence of induced second reflected wave with a small intensity is analysed instead of the secondary radiation yield within the total reflection domain for the first reflected wave.

Gleichungen zur Berechnung der Winkelabhängigkeit der sekundären Strahlungsausbeute (Photoelektronenemission oder Fluoreszenzstrahlung) unter den Bedingungen der dynamischen Röntgenmehrfachbeugung werden erhalten. Für eine geringe Ausbeutetiefe  $L_{yi}$  ist die Intensität der Sekundärstrahlung proportional zur Intensität der Röntgenstrahlen an den Atomplätzen einer Oberflächenschicht des Einkristalls. Wenn  $L_{yi} > L_A$ , wobei  $L_A$  die Röntgeneindringtiefe ist, ist die sekundäre Strahlungsintensität proportional zur gesamten absorbierten Energie der Röntgenstrahlen. Computersimulation des Dreiwellenfalles (444, 335, Bragg-Geometrie,  $\text{CuK}_\alpha$ , Si) zeigt, daß die Winkelabhängigkeit der Photoelektronenemissionsausbeute als repulsive Wechselwirkung zweier sich schneidender Zweiwellenmaxima beschrieben werden kann. Neue Möglichkeiten zur Beobachtung der stehenden Röntgenwellen im Zweiwellen-Fall werden diskutiert, wobei die Winkelabhängigkeit der zweiten induzierten reflektierten Welle mit einer geringen Intensität anstatt der sekundären Strahlungsausbeute innerhalb der Gesamt-Reflexionsdomäne für die erste reflektierte Welle analysiert wird.

### **1. Introduction**

The X-ray standing wave analysis of the subsurface layer of semiconducting crystals has been widely used in recent years (see, e.g., [1 to 6]). It consists in the registration of the angular dependence of the yield of secondary radiation (SR) such as photoelectron emission or fluorescence radiation, under the conditions of dynamical X-ray diffraction in single crystals. The amplitude  $E$  of the electric field of X-rays at an atomic site is the superposition of two plane waves: the entrance one  $E_0$  and the reflected one  $E_h$ . Within the angular domain of total reflection the amplitudes of these waves have nearly equal values. As a result a standing wave arises. The number of photoelectrons or fluorescence quanta emitted by atoms, is proportional to  $|E|^2$  and depends strongly on the phase of the relation  $E_h/E_0$ . That is why the angular dependence of the photoelectron emission differs essentially from the angular dependence of the X-ray reflection that is equal to  $|E_h|^2/|E_0|^2$ .

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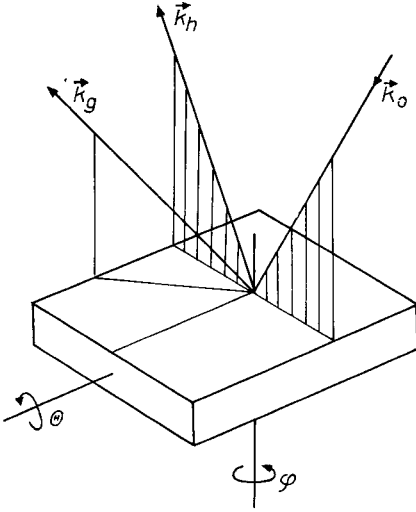


Fig. 1. The scheme of three-beam X-ray diffraction and the rotation axes of a crystal

The phase sensitivity of the X-ray standing wave method makes it very useful for studying the position of impurity atoms at the surface (adsorption) and in the bulk of a crystal near the surface. The method also allows to measure the displacements due to the crystal lattice relaxation after ion implantation or due to the incommensurability of lattice parameters in layer and substrate.

Up to now the nature of the arising X-ray standing wave and the motion of its nodes relative to the atomic planes with varying deviation from the Bragg angle is known well enough only for the two-beam case of X-ray diffraction. In the case of multiple diffraction the electric field which is the superposition of several plane waves, depends essentially on two mutually perpendicular angular deviations of the direction of the entrance beam from the direction that satisfies exactly several Bragg conditions. If the direction of the entrance beam is fixed, then the intensity of both reflected beams and the photoelectron emission change with crystal rotation around two axes, i.e. the axis  $\theta$  (rotation in the plane perpendicular to the crystal surface) and the axis  $\varphi$  (rotation in the surface plane), as is shown in Fig. 1.

The analysis of the two-dimensional angular dependence allows to localize two coordinates of an impurity atom site. Hence the measurement of SR yield under the conditions of multiple diffraction gives additional valuable information. In a single crystal one obtains the possibility to study the motion of two-dimensional stationary waves with the change of the entrance beam direction. To solve these problems it is necessary to develop further the theory of multiple X-ray diffraction. This is the aim of the present paper.

In the following section the derivation of the general equations is given. The specific example of the photoelectron emission in the case of three-beam (444, 335) diffraction of  $\text{CuK}_\alpha$  radiation in a Si single crystal is analyzed theoretically in Section 3. In Section 4 a new possibility of using two-wave standing waves without the measurement of SR yield is discussed in brief.

## 2. Derivation of General Equations

Let the crystal be oriented with respect to the entrance beam such that two Bragg conditions (or more in the presence of additional crystal symmetry elements) are satisfied simultaneously for reciprocal lattice vectors  $\mathbf{h}_m$ . Then the amplitude of the electric field in a crystal has the form

$$\mathbf{E}(\mathbf{r}, t) = e^{-i\omega t} \sum_{m=0}^{N-1} \mathbf{E}_m(z) e^{i\mathbf{k}_m \mathbf{r}}, \quad (1)$$

where  $N$  is the number of strong waves,  $\mathbf{k}_m = \mathbf{k}_0 + \mathbf{h}_m$ ,  $\mathbf{k}_0$  is the wave vector of the entrance wave,  $z$  the coordinate along an inner normal  $\mathbf{n}_0$  to the crystal surface. The transverse character of X-rays in a crystal is conserved because small additions of the order  $(1 - \varepsilon) \approx 10^{-5}$ , where  $\varepsilon$  is the dielectric function, can be neglected. Hence we may consider only two components of the vectors  $\mathbf{E}_m(z)$ , namely,

$$\mathbf{E}_m(z) = \sum_{s=\pi,\sigma} E_{ms}(z) \mathbf{e}_{ms}, \tag{2}$$

where  $\mathbf{e}_{m\pi}$  and  $\mathbf{e}_{m\sigma}$  are the unit polarization vectors for the  $m$ -th wave which are perpendicular both to  $\mathbf{k}_m$  and to each other.

The scalar amplitudes  $E_{ms}(z)$  satisfy a set of equations derived from the Maxwell equations. In this procedure we can neglect the second derivatives of the amplitudes with an error not exceeding  $(1 - \varepsilon)$ , if the parameters  $\gamma_m = \mathbf{k}_m \mathbf{n}_0 / |\mathbf{k}_m|$  are not too small. Then the set of equations has the form

$$\frac{2}{i} \frac{dE_{ms}}{dz} = \frac{2\pi}{\lambda \gamma_m} \sum_{m's'} [\chi_{mm'}^{ss'} - \alpha_m \delta_{mm'}^{ss'}] E_{m's'}. \tag{3}$$

Here  $\chi_{mm'}^{ss'} = \chi_{mm'}(\mathbf{e}_{ms} \mathbf{e}_{m's'})$  (in dipole approximation),  $\chi_{mm'}$  is the Fourier transform of the crystal polarizability  $\chi = \chi_r + i\chi_i$  with the reciprocal lattice vector  $\mathbf{h}_m - \mathbf{h}_{m'}$ ,  $\lambda$  the wavelength,

$$\alpha_m = \frac{k_m^2 - k_0^2}{\varkappa^2} = \alpha_{m1} \Delta\theta + \alpha_{m2} \Delta\varphi, \tag{4}$$

where  $\varkappa = 2\pi/\lambda = \omega/c$ . The  $\alpha_m$  parameters characterize the deviation from the Bragg conditions depending on  $\Delta\theta$ ,  $\Delta\varphi$ . Kronecker's symbol  $\delta_{mm'}^{ss'}$  is equal to unity if  $m = m'$  and  $s = s'$ .

Equations (1), (2) and the set of equations (3) are valid for a deformed crystal, too, provided the atomic displacements  $\mathbf{u}$  from the initial positions depend only on  $z$ . In this case it is necessary to use  $\tilde{\chi}_{mm'}^{ss'}$  instead of  $\chi_{mm'}^{ss'}$  where

$$\tilde{\chi}_{mm'}^{ss'} = \chi_{mm'}^{ss'} \exp [i(\mathbf{h}_{m'} - \mathbf{h}_m) \mathbf{u}(z) - W_{mm'}(z)]. \tag{5}$$

Here we introduce in addition the static Debye-Waller factor [8].

For a single crystal the set (3) has an analytical solution

$$E_{ms}(z) = \sum_{j=1}^{2N} \lambda_j E_{ms}(j) \exp \left[ (i\varepsilon_j - \mu_j) \frac{z}{2} \right], \tag{6}$$

where  $\varepsilon_j + i\mu_j$  and  $E_{ms}(j)$  are complex eigenvalues and eigenvectors for the matrix on the right-hand side of (3), the parameter  $\lambda_j$  are determined by the boundary conditions. In the case of  $N$  beams the matrix has the order  $2N \geq 6$ . Hence  $\varepsilon_j$ ,  $\mu_j$ , and  $E_{ms}(j)$  have no analytical expressions.

We are interested in the intensity of radiation at an atomic position  $\mathbf{r} = \mathbf{r}_A$  in the crystal. According to (1), (2), (6) it equals to

$$F(\mathbf{r}_A) = |\mathbf{E}(\mathbf{r}_A, t)|^2 = \sum_{jj'} A_{jj'} e^{-M_{jj'} z_A} \sum_{\substack{mm' \\ ss'}} E_{m's'}(j) E_{ms}^*(j') X_{mm'}^{ss'}(\mathbf{r}_A), \tag{7}$$

where the following notations are used:

$$\begin{aligned} A_{jj'} &= \lambda_j \lambda_{j'}^*, \\ M_{jj'} &= \frac{1}{2} (\mu_j + \mu_{j'} + i(\varepsilon_{j'} - \varepsilon_j)), \\ X_{mm'}^{ss'} &= (\mathbf{e}_{ms} \mathbf{e}_{m's'}) e^{i(\mathbf{h}_{m'} - \mathbf{h}_m) \mathbf{r}_A}. \end{aligned} \tag{8}$$

In experiment one determines an intensity of SR (e.g., of photoelectrons) which reaches the crystal surface. Consequently we must calculate the sum of (7) over the coordinates of all atoms and over all positions in which atoms move due to thermal vibrations. Moreover, we must account for the absorption of SR emitted in the depth  $z$  in the crystal bulk when they move towards the surface.

If SR is registered above the entrance surface of a crystal, then the intensity, averaged over atoms in the unit cell and the thermal vibrations, must be multiplied by

$$P(z) = e^{-\mu_{yi}z}, \quad (9)$$

where  $\mu_{yi}$  is the absorption coefficient of SR. For fluorescence radiation the exponential form of  $P(z)$  is exact, but in the case of photoelectron emission it is not [9]. However, for the sake of simplicity we shall use approximately (9) for this case, too.

The procedure of averaging over atoms in the unit cell and over thermal vibrations changes only the function  $X_{mm'}^{ss'}(\mathbf{r}_\lambda)$ . It is replaced by

$$\langle X_{mm'}^{ss'} \rangle = (\mathbf{e}_{ms} \mathbf{e}_{m's'}) \frac{1}{N_A} \sum_{n=1}^{N_A} e^{i(\mathbf{h}_{m'} - \mathbf{h}_m) \mathbf{r}_n} e^{-M_{mm'}^{(n)}(T)}, \quad (10)$$

where  $N_A$  is a number of atoms in a unit cell, and  $M_{mm'}^{(n)}(T) = 0.5(\mathbf{h}_m - \mathbf{h}_{m'})^2 \langle u_n^2 \rangle$ . The factor  $\exp(-M_{mm'}^{(n)})$  is the thermal Debye-Waller factor. The sum on the right-hand side of (10) is known as the structure factor. We note also that if one neglects weaker X-ray absorption processes than the photoelectric one, then

$$\langle X_{mm'}^{ss'} \rangle = \frac{\chi_{imm'}^{ss'}}{\chi_{i0}}, \quad (11)$$

where  $\chi_{imm'}^{ss'}$  is the imaginary part of the matrix which enters the set of equations (3).

Finally we have the following expression describing the angular dependence of SR yield:

$$\kappa(\Delta\theta, \Delta\varphi) = K \int_0^t dz P(z) \sum_{jj'} A_{jj'} e^{-M_{jj'} z} I_{jj'}, \quad (12)$$

where

$$I_{jj'} = \chi_{i0}^{-1} \sum_{\substack{mm' \\ ss'}} E_{m's'}(j) E_{ms'}^*(j') \chi_{imm'}^{ss'}, \quad (13)$$

$t$  is the crystal thickness,  $K$  a factor that does not depend on  $\Delta\theta$  and  $\Delta\varphi$ . Substituting (9) into (12) and integrating over  $z$  one obtains the expression

$$\kappa(\Delta\theta, \Delta\varphi) = L_0^{-1} \sum_{jj'} A_{jj'} L_{jj'} I_{jj'}, \quad (14)$$

where

$$L_{jj'} = \frac{1 - \exp(-(\mu_{yi} + M_{jj'})t)}{\mu_{yi} + M_{jj'}}, \quad (15)$$

$$L_0 = \frac{1}{\mu_{yi} + \mu_A}, \quad \mu_A = \frac{\mu_0}{\gamma_0}, \quad \mu_0 = \kappa \chi_{i0}. \quad (16)$$

In (14) the SR yield is normalized to its value in the absence of Bragg diffraction. If  $\mu_{yi}t \gg 1$ , then the quantity  $L_{jj'}$  does not depend on  $t$ . If, moreover,  $\mu_A t \gg 1$ , then in (14) it is necessary to account only for eigenvalues that correspond to  $\mu_j > 0$  and to find quantities  $\lambda_j$  from the boundary conditions only for the Laue beams ( $\gamma_m > 0$ ) [10, 11]. Thus, in a thick crystal the SR yield does not depend on its thickness.

Let us consider the case where  $L_{\text{ex}}\mu_{y1} \gg 1$ , and  $L_{\text{ex}}$  is the extinction depth. Then  $L_{jj'} \approx L_0$  and it follows from (14) that the function  $\kappa(\Delta\theta, \Delta\varphi)$  describes directly the angular dependence of the X-ray wave field intensity at the atom positions of a crystal subsurface layer.

Instead of (14) one may use also another formula which is derived with help of the relation

$$\mu_{\Lambda} I_{jj'} = M_{jj'} \Phi_{jj'}, \quad (17)$$

where

$$\Phi_{jj'} = \sum_{ms} E_{ms}^*(j') E_{ms}(j) \frac{\gamma_m}{\gamma_0}. \quad (18)$$

The derivation of (17) in the case  $j = j'$  has been done in [12]. A more general equation with  $j \neq j'$  is derived similarly in [13]. As a result the equivalent expression for  $\kappa(\Delta\theta, \Delta\varphi)$  may be written in the form

$$\kappa(\Delta\theta, \Delta\varphi) = (\mu_{\Lambda} L_0)^{-1} \sum_{jj'} A_{jj'} L_{jj'} M_{jj'} \Phi_{jj'}. \quad (19)$$

Equation (19) is more suitable for a computer simulation because  $\Phi_{jj'}$  involves only one sum over  $ms$  instead of the double sum in  $I_{jj'}$ .

Consider now the case, where  $\mu_{y1} < M_{jj'}$ , but  $\mu_{\Lambda} t \gg 1$  (thick crystal). Then  $L_{jj'} M_{jj'} \approx \approx 1$  and in accordance with (19) the angular dependence of the SR yield is described approximately by the expression

$$\kappa(\Delta\theta, \Delta\varphi) \approx \sum_{jj'} A_{jj'} \Phi_{jj'} = 1 - \sum_{\substack{ms \\ \gamma_m < 0}} R_{ms}, \quad (20)$$

where  $R_{ms}$  is the X-ray reflection coefficient for the  $s$ -th polarization state,

$$R_{ms} = \left| \sum_j \lambda_j E_{ms}(j) \right|^2 \frac{|\gamma_m|}{\gamma_0}. \quad (21)$$

The right-hand side of (20) is a consequence of the boundary conditions and of the definition of  $R_{ms}$ .

The expression obtained has a simple physical meaning. When the SR yield depth becomes greater than the X-ray penetration depth, the SR intensity is proportional to the total absorbed energy of X-rays in the crystal. Such a situation is realized, as a rule, when one registers the fluorescence radiation.

### 3. Analysis of the Specific Case Three-Beam (444, 335) Diffraction of CuK $_{\alpha}$ Radiation in Si

The above-obtained equations can be used for an analysis of the angular dependence of SR yield under conditions of multiple X-ray diffraction with arbitrary number of both Laue beams ( $\gamma_m > 0$ ) and Bragg beams ( $\gamma_m < 0$ ). As an example, in this section we consider the photoelectron emission in Si under the conditions of three-beam (444, 335) diffraction of CuK $_{\alpha}$  radiation ( $\lambda = 0.154$  nm). The reciprocal lattice vectors 444 and 335 are denoted as  $\mathbf{h}$  and  $\mathbf{g}$ . In this particular case they are nearly parallel and make an angle of 14.5°. Moreover, the wave vectors  $\mathbf{k}_0$ ,  $\mathbf{k}_h$ , and  $\mathbf{k}_g$  for the given wavelength are nearly in the plane of the vectors  $\mathbf{h}$  and  $\mathbf{g}$ . It is easy to understand with account of this facts that all polarization factors are approximately equal to unity. As a result both the intensity of the photoelectron emission  $\kappa(\Delta\theta, \Delta\varphi)$  and the X-ray reflection coefficients  $R_m(\Delta\theta, \Delta\varphi)$ ;  $m = h, g$ , depend weakly on the polarization state of the incident radiation. This fact has been confirmed by a numerical computation.

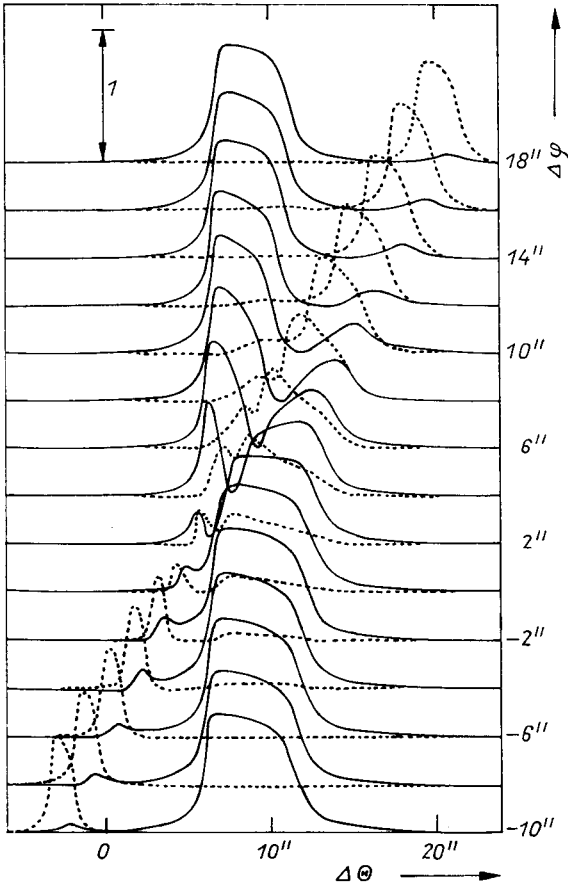


Fig. 2. The curves of  $\Delta\theta$ -dependence of X-ray diffraction reflection coefficients for different values of  $\Delta\varphi$  in the case of three-beam (444, 335) diffraction of  $\text{CuK}_\alpha$  radiation in Si. Solid lines 444, dotted lines 335. The angular deviations  $\Delta\theta$ ,  $\Delta\varphi$  are given in seconds of arc ( $1'' = 0.485 \times 10^{-5}$  rad)

Fig. 2 and 3 show the computational results for a nonpolarized, ideally collimated beam. The crystal surface is normal to the vector  $\mathbf{h}$ . For the rotation axes used (angles  $\theta$  and  $\varphi$ , see Fig. 1) the Bragg condition for the vector  $\mathbf{h}$  (parameter  $\alpha_h$ ) does not depend on  $\Delta\varphi$ . As a result the region of total diffraction reflection (RTDR) for the  $\mathbf{h}$ -beam has the form of a stripe parallel to the axis  $\varphi$  on the plane of the angular deviations  $\Delta\theta$ ,  $\Delta\varphi$ . The angle between the axis  $\varphi$  and the RTDR stripe of the  $\mathbf{g}$ -beam is  $36.8^\circ$ . It is known [7] that the value of the section of two-beam RTDR with the  $\theta$ -axis is equal to  $x_m = 4\beta_m^{-1/2}|\chi_m|/|\alpha_{m1}|$ , where  $\beta_m = \gamma_0/|\gamma_m|$  and  $\alpha_{m1}$  is a coefficient in (4). The displacement of a RTDR centre from the point  $\Delta\theta = 0$  on the line  $\Delta\varphi = 0$  is equal to  $\Delta\theta_m = -|\chi_0|(1 + \beta_m)/\beta_m\alpha_{m1}$ . In the case considered these parameters have the values  $x_m = 5.24''$  and  $2.32''$ ,  $\Delta\theta_m = 8.58''$  and  $5.22''$  for reflection 444 and 335, respectively.

According to Fig. 2 and 3 the angular dependence of  $\kappa$  and  $R_m$  can be described as an interaction of the two-beam RTDR due to their crossing. Let us consider the change of the form of RTDR along the  $\theta$ -axis with varying value of  $\Delta\varphi$ . For large values of  $\Delta\varphi$  when the distance between RTDR  $L(\Delta\varphi) \gg x_m$  their interaction can be accounted for perturbatively [14, 15]. Then the equations of the two-beam approximation are conserved but only with renormalized values of the parameters  $\chi_{mm'}$ . For example, in

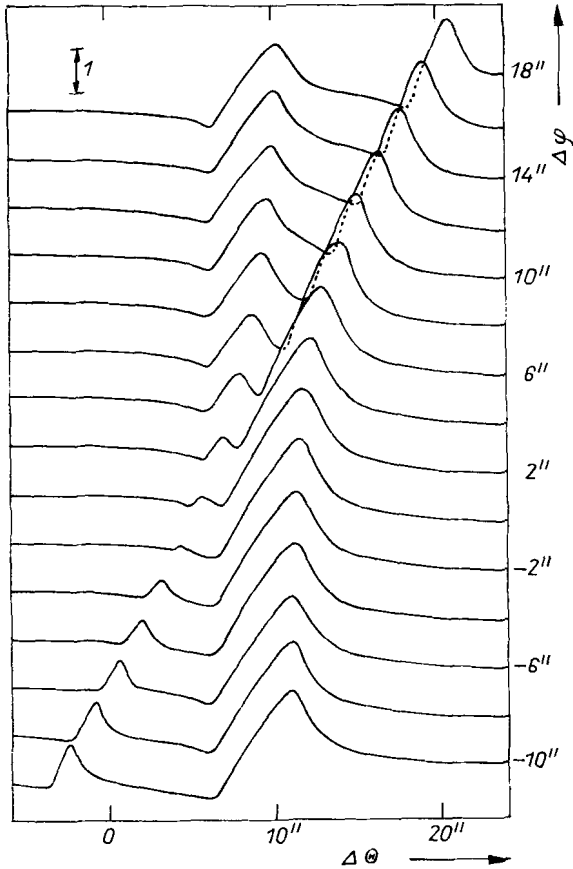


Fig. 3. The curves of  $\Delta\theta$ -dependence of the photoelectron emission for different values of  $\Delta\varphi$  in the same case, as in Fig. 2

the  $h$ -beam

$$\chi_h = \chi_{h0} \rightarrow \chi_{h0} + \frac{\chi_{hg}\chi_{g0}}{C_g \Delta\varphi}, \tag{22}$$

where  $C_g$  is a coefficient. Accordingly such parameters of RTDR as width and centre displacement also change asymmetrically with respect to the sign of  $\Delta\varphi$ .

It is easy to see in Fig. 2 that RTDR for the  $h$ -beam become narrow and move to the left on the side  $\Delta\varphi > 0$  from the multiple region and vice versa. The RTDR for the  $g$ -beam becomes narrow on the side  $\Delta\varphi < 0$ . Therefore, the existence of two maxima of X-ray reflection for each beam in the central part of the many-beam region is a natural consequence of this behaviour. In fact, two maxima exist also for  $\Delta\varphi$  values which correspond to  $L(\Delta\varphi) > x_m$ . The reason for this can be understood if one considers, e.g., the equation for the amplitude  $E_g$ . Neglecting, for the sake of simplicity, polarization effects one obtains easily from (3), (6) the expression for the amplitude

$$E_g = \frac{\kappa[\chi_{g0}E_0 + \chi_{gh}E_h]}{\gamma_g\varepsilon - \kappa\chi_0 + \kappa\alpha_g}, \tag{23}$$

where  $\varepsilon = \varepsilon + i\mu$  is a complex eigenvalue.

According to (23) the maximum of  $E_g$  with a change of  $\Delta\theta$  can appear under two conditions. Firstly, it arises when the Bragg condition for the  $g$ -beam is satisfied ( $\alpha_g = 0$ ), then the denominator of (23) decreases. Secondly, when the Bragg condition for the  $h$ -beam is satisfied ( $\alpha_h = 0$ ), then the numerator of (23) increases sharply with

the increase of the amplitude  $E_h$ , and the second maximum arises. This becomes weak with increasing  $L(\Delta\varphi)$ , when  $\alpha_g$  grows. Hence, the first and second maxima can be called the proper maximum and induced maximum, respectively. At the point of intersection of two-beam stripes of RTDR the proper maximum transforms into the induced one and the two-beam stripe breaks off. It is interesting that in the multiple diffraction angular region there are areas where the sum of X-ray reflection coefficients has a value that is smaller than unity. In other words, the total reflection effect does not exist under the conditions of three-beam diffraction.

The intensity of photoelectron emission has contributions from all beams. As a result, the angular dependence of the photoeffect (Fig. 3) has two equivalent maxima for all values of  $\Delta\varphi$ . We used in the calculations (19). In a given case the yield depth of the photoelectron emission is  $L_{yi} = 0.46 \mu\text{m}$  [9]. Following [15] we used  $P(z)$  in the exponential form with  $\mu_{yi} = 2.3/L_{yi} = 5 \mu\text{m}^{-1}$ .

Fig. 3 shows that the total radiation field at the atoms of a crystal depends on  $\Delta\theta$  as in the two-beam case (see, e.g., [1, 2]). Such an angular dependence takes place practically for all values of  $\Delta\varphi$ , but the amplitude of the intensity change depends strongly and asymmetrically on  $\Delta\varphi$ . The change of two maxima in Fig. 3 with decreasing distance between them can be characterized as a repulsion. The left maximum becomes weaker with decreasing distance. For the minimum distance it almost vanishes though the sum of X-ray reflection coefficients does not equal zero for the given angle values. Therefore, this effect has interference character.

The reciprocal lattice vector  $\mathbf{g}$  has a nonzero projection along the crystal surface. Thus, one can obtain a structural information about the crystal in both directions normal and parallel to the surface through analysing the two maxima.

#### 4. X-Ray Standing Wave Method without Secondary Radiation

In this section we want to show a new possibility for the observation of X-ray standing waves in the intensity of the induced maximum of X-ray reflection. According to (23), for large values of  $\alpha_g$  we have

$$I_g = |E_g|^2 \approx \frac{|\chi_{g0}|^2}{\alpha_g^2} \left| E_0 + \frac{\chi_{gh}}{\chi_{g0}} E_h \right|^2. \quad (24)$$

In the RTDR for the  $h$ -beam the angular dependence of the  $g$ -beam intensity contains information about the phase of the ratio  $E_h/E_0$ . Because  $\alpha_g$  has a large value, the  $g$ -beam is weak and does not practically influence the amplitudes  $E_0$  and  $E_h$ . Therefore, they have the values of the two-beam approximation. It follows from (24) that the angular dependence of the induced maximum differs essentially from that of the proper maximum. This fact has been observed clearly in experiments [17, 18]. On the other hand, the intensity of the  $h$ -beam depends on the phase of the ratio  $E_g/E_0$  within the RTDR for a  $g$ -beam.

Moreover, this method can be used in an analysis of the structure of distorted surface layers. If the atoms near the surface are displaced from the regular positions, then the parameters  $\chi_{mm'}$  have additional phase factors as follows from (5). Taking into account also the polarization factors we have the following expression for the intensity of the induced beam in the case of a polarized entrance beam ( $s = \pi, \sigma$ ):

$$I_g^s = \frac{|\chi_{g0}|^2}{\alpha_g^2} I_0^s \left\{ \left( \mathbf{e}_{g\sigma} \mathbf{e}_{0s} \right) + \frac{\chi_{gh}}{\chi_{g0}} e^{i\mathbf{h}\mathbf{u}(0)} \left( \mathbf{e}_{g\sigma} \mathbf{e}_{hs} \right) \frac{E_{hs}}{E_{0s}} \right\}^2 + \left\{ \left( \mathbf{e}_{g\pi} \mathbf{e}_{0s} \right) + \frac{\chi_{gh}}{\chi_{g0}} e^{i\mathbf{h}\mathbf{u}(0)} \left( \mathbf{e}_{g\pi} \mathbf{e}_{hs} \right) \frac{E_{hs}}{E_{0s}} \right\}^2, \quad (25)$$

where  $\mathbf{u}(0)$  is the displacement of an atomic plane on the surface of a crystal.



Now the angular dependence on  $\Delta\theta$  allows to determine the phase  $hu(0)$  in addition to the phase of  $E_h/E_0$ . Consequently we may characterize the degree of crystal lattice deformation in the subsurface layer as in the X-ray standing wave method in the case of photoelectron emission. However, in a given case there is no necessity to measure SR. It can be shown that the thickness of the subsurface layer which is analysed by this method is very small and it tends to zero with increasing  $\alpha_p$ .

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