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*Institute of Nuclear Problems, Belorussian State University, Minsk<sup>1)</sup>*

## **Effect of Two Critical Angles of X-Ray Surface Diffraction on Secondary Emission Yield**

By

V. G. BARYSHEVSKII and S. A. STEPANOV

The dependence of secondary fluorescence yield from the crystal on the angle of incidence of an X-ray beam under conditions of surface diffraction is theoretically studied. It is shown, that location of surface deposited impurity atoms in the crystal matrix may be determined from the shape of secondary emission curves.

Теоретически исследована зависимость интенсивности выхода вторичного излучения из кристалла от угла падения рентгеновского пучка в условиях поверхностной дифракции рентгеновских лучей. Показано, что форме вторично-эмиссионных кривых можно определять положение в решетке кристалла примесных атомов, осажденных на его поверхности.

### **1. Introduction**

X-ray surface diffraction [1 to 3] has been actively studied in last years as it is a promising instrument for investigating a crystal surface.

In particular, in works [4 to 6] the variation of the yield of the fluorescent quanta and photoelectrons under surface diffraction conditions were investigated. It was shown, that secondary emission provides information on the structure of an X-ray wave field in a crystal, particularly in those cases, where a diffracted wave cannot be recorded experimentally because of the total internal reflection effect.

The authors [4 to 6] restricted themselves to the analysis of curves of secondary emission yield, averaged over the contributions of all the atoms in a crystal. It was noted in [6], that the averaged secondary emission curves do not give, in principle, more information compared to those of X-ray diffraction, since the escape depth of most secondary radiations exceeds that of formation of an X-ray standing wave field under surface diffraction.

In this connection we think, that under conditions of surface diffraction, the most interesting thing is a record of a characteristic fluorescence not from all of the crystal matrix, but from impurity atoms, deposited in this or that way on its surface, what deliberately fixes the small escape depth. The suggested approach is similar to that, advanced in [7] for the Bragg-case geometry of X-ray diffraction. It will be shown below, that it allows one to determine location of impurity atoms in a crystal lattice.

### **2. Derivation of the Basic Equations**

Consider a fluorescent atom, located at a depth of  $z$  at a point with coordinate  $\varrho_{\perp}$ , taken along the surface. The fluorescence intensity of this atom in a crystal is proportional to the

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<sup>1)</sup> Bobruiskaya, SU-220 050 Minsk, USSR.

module square  $|D(z, \boldsymbol{q}_\perp)|^2$  of the X-ray electric field strength at a location of the atom. In order to obtain the fluorescence intensity in vacuum in front of the crystal surface, it is necessary to multiply the emission intensity of the atom by the probability of the fluorescent quanta escape from the depth  $z$ . Owing to a small depth of location of fluorescent atoms in the case under consideration, the escape probability may be assumed to be equal to unity. Thus, in particular case of surface diffraction of  $\sigma$ -polarized incident waves we have (see [8] for details)

$$I_{\text{flu}}(\varphi_0, \alpha, z, \boldsymbol{q}_\perp) \sim \left| \sum_{j=1}^2 (D_0^{(j)} + D_h^{(j)} e^{i\boldsymbol{h}\boldsymbol{e}_\perp + i\boldsymbol{\kappa}_0\boldsymbol{\psi}z} e^{i\boldsymbol{\kappa}_0 u^{(j)}z}) \right|^2. \quad (1)$$

Here  $D_{0,h}^{(1,2)} \equiv D_{0,h}^{(1,2)}(\varphi_0, \alpha)$  are the amplitudes of two transmitted and two diffracted waves constituting the wave field in a crystal under surface diffraction. They take on the form

$$D_0^{(j)} = \frac{2(-1)^{3-j} W^{(3-j)} (u^{(3-j)} + \varphi_h + \psi)}{W^{(2)} (u^{(2)} + \varphi_h + \psi) (u^{(1)} + \varphi_0) - W^{(1)} (u^{(1)} + \varphi_h + \psi) (u^{(2)} + \varphi_0)}. \quad (2)$$

$$D_h^{(j)} = \frac{W^{(j)}}{\chi_h} D_0^{(j)}, \quad (3)$$

$\boldsymbol{h}$  is the reciprocal lattice vector,  $\boldsymbol{\kappa}_0$  is the wave vector of an incident X-ray wave,  $\varphi_0$  is the angle of incidence,  $\psi$  is the effective disorientation angle of the reciprocal lattice vector relative to the surface,  $\alpha$  is the Bragg deviation parameter,  $\varphi_h$  is the angle of exit from the crystal of a diffracted X-ray wave ( $\varphi_h^2 = (\varphi_0 + \psi)^2 - \alpha$ ),  $\chi_0$ ,  $\chi_h$ ,  $\chi_{\bar{h}}$  are the crystal polarizabilities,  $W^{(j)} = u^{(j)2} - \varphi_0^2 - \boldsymbol{\kappa}_0$ ,  $u^{(j)}$  are the two roots with  $\text{Im}(u^{(j)}) > 0$  of the following dispersion equation:

$$(u^2 - \varphi_0^2 - \chi_0) ((u + \psi)^2 - \varphi_h^2 - \chi_0) = \chi_h \chi_{\bar{h}}. \quad (4)$$

Expanding the square of module in (1), we obtain

$$\begin{aligned} I_{\text{flu}}(\varphi_0, \alpha, z, \boldsymbol{q}_\perp) \sim & \sum_{j=1}^2 [ |D_0^{(j)}|^2 + |D_h^{(j)}|^2 ] a^{(j)} + 2 \text{Re}[(D_0^{(1)} D_0^{(2)*} + D_h^{(1)} D_h^{(2)*}) b] \\ & + 2 \sum_{j=1}^2 \text{Re}[D_0^{(j)} D_h^{(j)*} a^{(j)} c(x)] + 2 \text{Re}[(D_0^{(1)} D_h^{(2)*} b + D_0^{(2)} D_h^{(1)*} b^*) c(x)], \end{aligned} \quad (5)$$

where  $x$  is the component of  $\boldsymbol{q}_\perp$  along the vector  $\boldsymbol{h}$ ,

$$a^{(j)} = e^{-2\boldsymbol{\kappa}_0 \text{Im}(u^{(j)})z}, \quad b = e^{i\boldsymbol{\kappa}_0(u^{(1)} - u^{(2)*})z}, \quad c(x) = e^{-i\boldsymbol{h}x - i\boldsymbol{\kappa}_0\boldsymbol{\psi}z}.$$

### 3. Discussion

As follows from (5), the fluorescence intensity is composed of two contributions. The first contribution (terms 1 and 2) does not depend on  $x$ . And the second one (terms 3 and 4), on the contrary, is sensitive to the position of a fluorescent atom with respect to diffracting planes. It is obvious, that the presence of the contribution, which depends on  $x$ , permits one to locate an atom in a crystal lattice by the shape of a fluorescence curve.

Consider for certain a particular case, that is the incidence angle dependence of the fluorescence yield from the crystal surface ( $z = 0$ ) at  $\alpha = 0$  and  $\psi = 0$ . From (2) and (3) we

have

$$D_0^{(j)} = (-1)^{3-j} D_h^{(j)} = \frac{\varphi_0}{u^{(j)} + \varphi_0}, \quad (6)$$

where

$$u^{(1,2)} = (\varphi_0^2 + \chi_0 \pm \chi_h)^{1/2}.$$

Substituting (6) into (5), one may obtain

$$I_{\text{flu}}(\varphi_0, x) \sim 2(|D_0^{(1)}|^2 + |D_0^{(2)}|^2) + 2(|D_0^{(1)}|^2 - |D_0^{(2)}|^2) \cos(hx). \quad (7)$$

Thus,

$$I_{\text{flu}}(\varphi_0) \sim 4|D_0^{(1)}|^2 \quad (8a)$$

at  $hx = 0, 2\pi, \dots$ , when fluorescent atoms lie on diffracting planes;

$$I_{\text{flu}}(\varphi_0) \sim 4|D_0^{(2)}|^2 \quad (8b)$$

at  $hx = \pi, 3\pi, \dots$ , when fluorescent atoms lie in the middle between diffracting planes;

$$I_{\text{flu}}(\varphi_0) \sim 2(|D_0^{(1)}|^2 + |D_0^{(2)}|^2) \quad (8c)$$

at a random arrangement of fluorescent atoms (when averaging is made over  $x$ ).

Corresponding plots are given in Fig. 1 (curves 1 to 3). Dashed line (curve 4) shows the incidence angle dependence of the surface fluorescence yield when the X-ray beam is specularly reflected from the surface outside Bragg diffraction conditions.

The equations and figures given above have a simple physical explanation. They testify to the existence of two X-ray standing waves in a crystal under surface diffraction. These waves have strong and weak amplitudes of interaction with matter and, respectively, different critical angles of total external reflection (see [1, 9, 10]). For a fluorescent atom, located on diffraction planes, the total irradiation X-ray intensity is completely defined by a strongly interacting field, forming antinodes on these planes. And contrary to this, an atom, located in the middle between the planes, is irradiated only by a weakly interacting X-ray field.

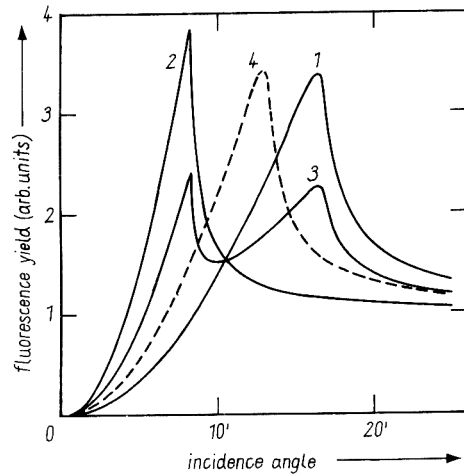


Fig. 1. Fluorescence yield from Si crystal surface as a function of the incident angle of an X-ray beam under surface diffraction of  $\text{CuK}\alpha_1$  radiation on (220) planes. Fluorescent atoms are (1) in sites, (2) in interstitials, (3) distributed uniformly throughout the lattice, (4) no diffraction

As follows from (6), fluorescent curves in Fig. 1 show maximum intensity at the angle of incidence, which is equal to the critical angle of total external reflection for the respective field:  $\varphi_0 = (|\chi_o| + |\chi_h|)^{1/2}$  for curve 1,  $\varphi_0 = (|\chi_o| - |\chi_h|)^{1/2}$  for curve 2 and  $\varphi_0 = (|\chi_o|)^{1/2}$  for curve 4.

#### 4. Conclusions

Thus, location of impurity atoms in lattice along the crystal surface may be determined from the angular position of a maximum on the curves of fluorescence yield under conditions of surface diffraction.

Choice of two nonparallel reciprocal lattice vectors, corresponding to surface diffraction, provides two coordinates of impurity atoms along the surface.

According to (5), depth  $z$  may also be determined in addition to the data of method [7], since in [7] not the depth of impurity location is measured, but its displacement with respect to atomic planes, parallel to the surface.

In conclusion, we should note, that according to [11], in the multi-beam case of surface diffraction there are more than two thresholds of total specular reflection. As a consequence, the number of maxima in the secondary emission yield is growing in this case.

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