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Institute of Nuclear Problems, Belorussian State University, Minsk[1])

On Disagreements between Theory and Experiment in X-Ray Grazing Incidence Diffraction

By
S.A. STEPANOV

Introduction Studies in the field of X-ray grazing incidence diffraction (GID), stimulated by the notable work /1/, are actively developed because of its promising applications for controlling crystal surfaces. However, experimental tests /2 to 5/ intended to verify the dynamical theory of GID /7 to 9/, did not so far clarify completely the validity of this theory. In particular:

1. The most thorough study /5/ revealed systematic deviations of experimental curves in the direction of a higher azimuthal angle θ with increasing angle of incidence ϕ of the X-ray beam to the crystal surface.

2. None of the works showed a sharp peak at $\alpha = 0$ and $\phi = \sqrt{|\chi_o - \chi_h|}$ on diffraction curves taken under GID conditions (α is the parameter of deviation from the Bragg condition, χ_o, χ_h are the crystal polarizabilities).

In the present note, we propose an explanation of the "systematic deviation" effect, and outline the idea of an experiment for the observation of sharp peaks on GID curves.

Systematic angular deviations We assume that "systematic deviations" are associated with a simple, but earlier ignored fact, that in a GID geometry the parameter α depends not only on the azimuthal angle θ, but also on ϕ. Indeed, in previous works one could find the following equation for α:

$$\alpha = \frac{2\vec{\kappa}_o\vec{h} + h^2}{\kappa_o^2} = -2\sin(2\theta_B)(\theta_x - \theta_B) \quad , \tag{1}$$

where $(90^o - \theta_x)$ is the angle between the incident wave vector $\vec{\kappa}_o$ and the reciprocal lattice vector $\vec{h}$. The angle θ_x was assumed to be the azimuthal scanning angle. We have taken into account that θ_x varies in a plane, slightly inclined towards the surface (see Fig. 1), whereas experimental measurements are taken with respect to angles ϕ and θ, varying in two mutually perpendicular planes - the plane of incidence and the surface plane. Therefore the parameter α should be expressed in terms of θ, and not in terms of θ_x. From Fig. 1 we obtain

[1]) Bobruiskaya 11, SU-220050 Minsk, USSR.

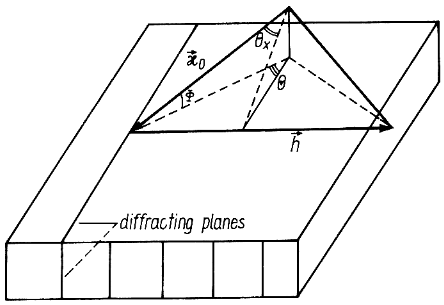

Fig. 1. Grazing incidence diffraction geometry with schematic illustration of scanning angles. $\vec{\kappa}_o$ incident wave vector, $\vec{h}$ reciprocal lattice vector, ϕ angle of incidence, θ azimuthal scanning angle, θ_x "old" azimuthal scanning angle

$$\theta_x \approx \theta - \frac{\phi^2}{2} \tan(\theta_B) \quad , \tag{2}$$

$$\alpha = -2 \sin(2\theta_B)(\theta - \theta_B) + 2\phi^2 \sin^2(\theta_B) \ . \tag{3}$$

From (3) immediately follows that α depends not only on θ, but also on ϕ. In spite of the fact that the former dependence is linear and the latter is a square one, scannings in θ and ϕ provide contributions to α of the same order, since ranges of these scannings considerably differ: $\Delta\theta \approx 10^{-5}$ to 10^{-4} rad and $\Delta\phi \approx 10^{-3}$ to 10^{-2} rad.

In Fig. 2a, b theoretical GID curves, simulating the experiment in /5/ (Ge(220), 7.9 keV) are presented. Fig. 2a shows computations performed as in /5/, i.e. with no account for the second term in (3). Fig. 2b gives the same evaluations with application of (3). One can easily see that the tail of a curve in Fig. 2b is shifted towards the right by $\approx 5''$, which coincides completely with the experiment in /5/.

In a more general case of GID where the reciprocal lattice vector $\vec{h}$ is disoriented from the surface by the angle ψ (see /9/), (3) takes a more complex form:

$$\alpha = -2 \sin(2\theta_B)(\theta - \theta_B) + 2(\phi^2 + \psi^2)\sin^2(\theta_B) + 4\phi\psi \sin(\theta_B) \quad . \tag{4}$$

Note, that the corrections we have obtained for the angular dependence of the parameter α, play an important role in the surface Bond method based on GID, suggested in /10/.

Registration of a sharp maximum We suppose that the absence of narrow maxima in experimental GID curves at an incident angle $\phi = \sqrt{|\chi_o - \chi_h|}$ is explained by a rather small angular width of these peaks in θ: $\Delta\theta \leqq 0.5$ which is by an order of magnitude less than X-ray monochromators usually provide. In this connection, it would be advisable to verify the dynamical theory of GID near the back diffraction conditions ($\theta_B \approx 90^o$). Under these conditions, the angular dependence $\alpha(\theta)$ becomes a square law /11, 12/ and the peak width

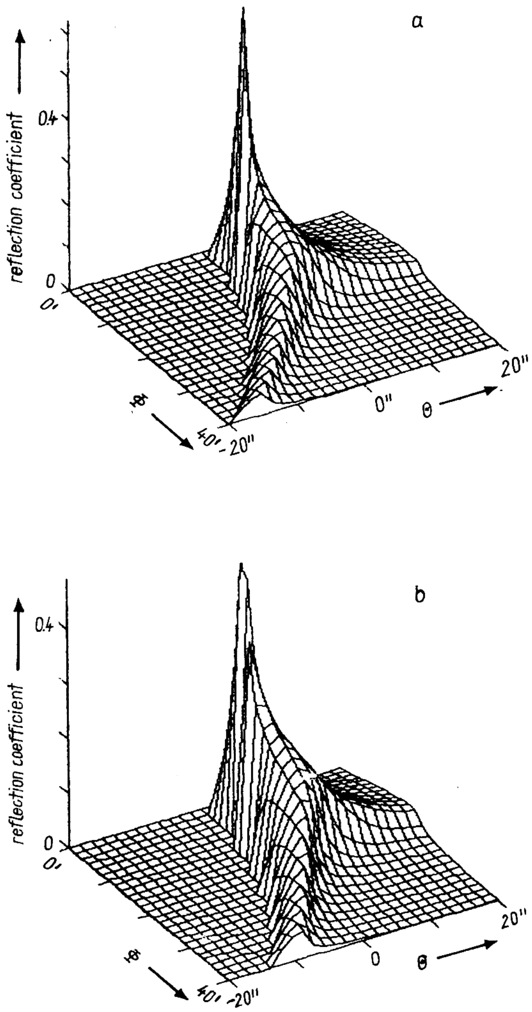

Fig. 2. Theoretical dependence of the diffracted wave reflection coefficient taken on angles ϕ and θ under GID conditions. a) Previous works, b) corrected according to (3)

in θ increases by two orders. An experimental scheme to study grazing incidence back diffraction has been worked out in /12/. However, to make a precise verification of the theory, measurements are to be taken on a super clean crystal surface under high vacuum, as GID curves are extremely sensitive to surface distortions in this region.

In conclusion, the author would like to express his readiness to cooperate with all colleagues, who show interest in implementation of experiments proposed.

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