

DEVELOPMENT OF THE COMPLEX METHODS FOR NUMERICAL CALCULATIONS OF DOUBLE- AND MULTI-CRYSTAL ROCKING CURVES



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Introduction

X-rays have been proven to be a powerful and reliable tool in studying a large diversity of micro- and nanoscale objects. The wavelength of X-rays is a perfect fit to the typical sizes of basic structures used in all modern technologies and science: crystallographic lattice in semiconductor thin films; biological molecules in protein crystallography; nanoscale objects like quantum dots and quantum wires in optoelectronics; and many others. This fact initiated the intensive development of various measurement techniques and instrumentation to satisfy the large variety of requirements coming from scientific and industrial communities. Information on the intrinsic structure of samples is further obtained from the detailed analysis of the scattered and detected X-ray intensities, which demands robust theoretical methods for rocking curves interpretation.

Double-crystall diffractionometry (DCD)

Currently, the method of measuring and analyzing RCs is one of the main highly sensitive tools for nondestructive diagnostics of the structural quality of crystalline materials, in particular, the volume and surface defects in single crystals, thin films, and multilayer crystal structures.

Double-crystal rocking curve (RC) is a narrow (on the order of few arcsec) line with a half-width somewhat exceeding the half-width of the so-called “intrinsic” RC, to which the monochromator crystal and sample are tuned. At the same time, it was shown in [1,2] that considering the instrumental function of a double-crystal diffractometer, which includes the spectral distribution of the incident characteristic X-rays from the tube and takes into account the influence of slit collimators used to select the fundamental characteristic line, leads to an additional contribution from the neighboring characteristic X-ray line in the RC under consideration.

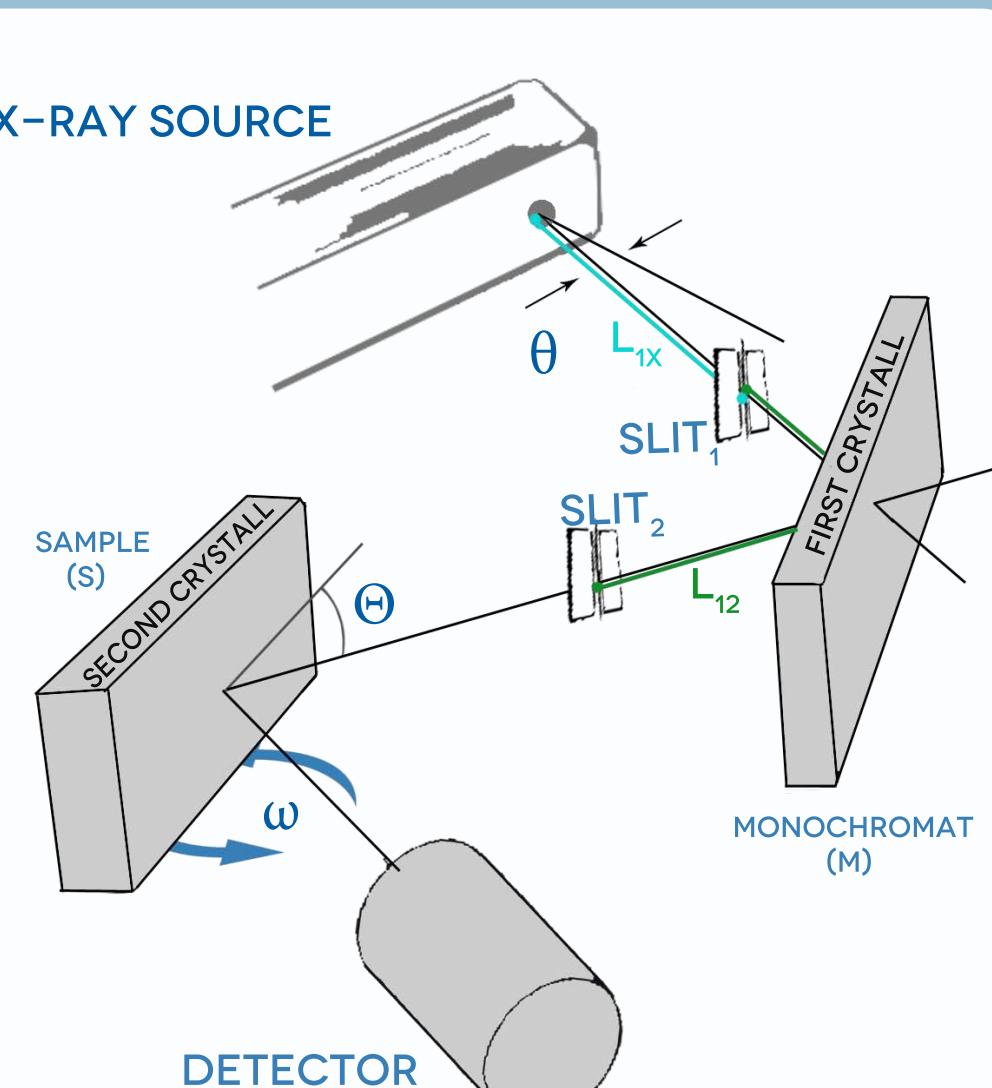


Figure 1: DCD experimental scheme

For a double-crystal diffractometer, the expression for RC:

$$I(\omega) = I_0 \cdot \iint d\theta d\lambda g_\lambda(\lambda) g_\theta(\theta) R_M \left(\theta - \frac{\lambda - \lambda_1}{\lambda_1} \tan \Theta_B \right) \cdot R_S \left(\omega + \theta - \frac{\lambda - \lambda_1}{\lambda_1} \tan \Theta_B \right) \quad (1)$$

The instrumental function [2]:

$$g_\theta(\theta) = \frac{1}{\int g_\theta(\theta)d\theta} \int_{x_1(\theta)}^{x_2(\theta)} e^{-x^2} dx \quad (2)$$

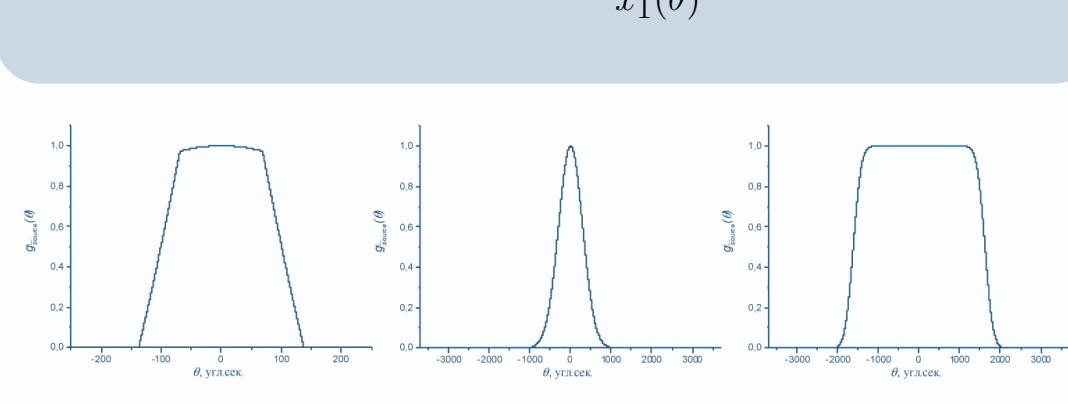


Figure 2: Instrumental function

It is of importance: we should note that the theoretical approach to calculating double-crystal RCs in the nondispersive (or not) scheme is also valid for X-ray tubes with anodes made of other materials (copper, tungsten, etc.).

For the result:

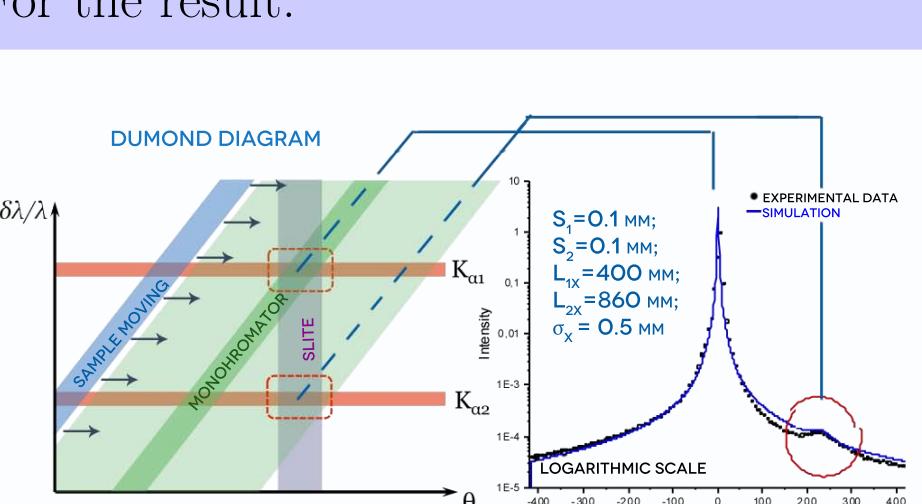


Figure 3: DuMond diagram and rocking curve of double crystal diffraction scheme

Spectral function is a superposition of two narrow characteristic X-ray lines:

$$g_\lambda(\lambda) = \frac{2}{3\pi} \left\{ \frac{\delta\lambda_1}{(\lambda - \lambda_1)^2 + (\delta\lambda_1)^2} + \frac{1}{2} \frac{\delta\lambda_2}{(\lambda - \lambda_2)^2 + (\delta\lambda_2)^2} \right\} \quad (3)$$

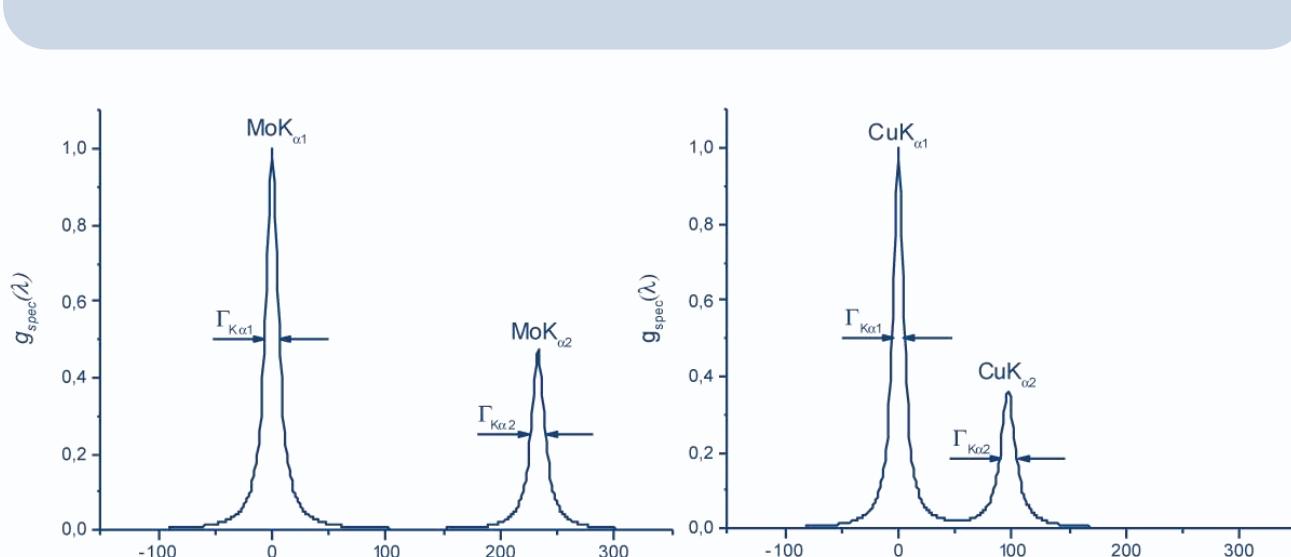


Figure 4: X-Ray spectrum function

Scheme in which there is a difference between Bragg angles of monochromator (M) and specimen (S) is named as a dispersive scheme:

$$FWHM_{RC} = FWHM_M^2 + FWHM_S^2 + \left[\frac{\Delta\lambda}{\lambda} (tg(\Theta_{BS}) - tg(\Theta_{BM})) \right]^2, \quad (4)$$

where FWHM - full width at half maximum;
 $\frac{\Delta\lambda}{\lambda} = 3 \cdot 10^{-4}$.

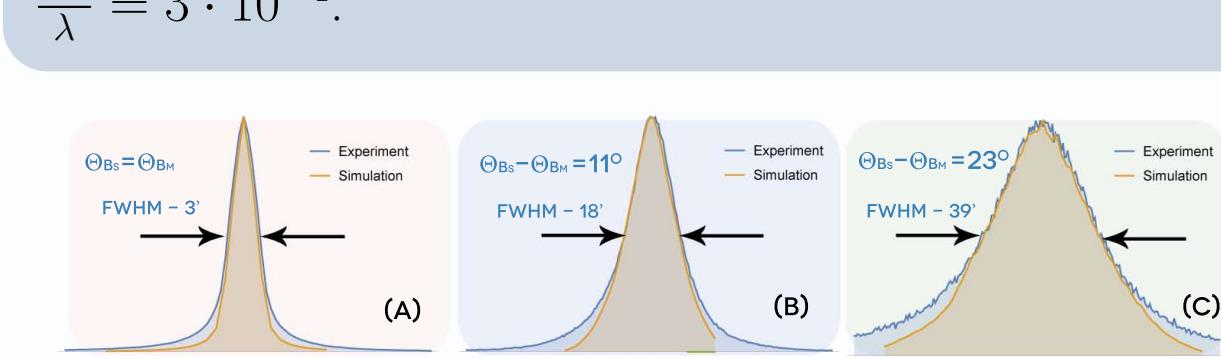


Figure 5: Double crystal rocking curve for monochromator Si[220] and sample: A) Si[220]; B) Si[440]; C) Si[660]

Triple-crystall diffractionometry (TCD)

Triple crystal diffractometry has proved to be an important method for investigations of imperfections in crystals. The angular separation of dynamical and kinematical diffracted intensities is one advantage of this method. The other is the possibility to investigate the diffuse scattering of imperfections very close to the Bragg peak and to show this as equi-intensity contours near the reciprocal lattice point. Thus, it is possible to determine the strain field of defects.

For a triple-crystal diffractometer, the expression:

$$I(\varepsilon, \omega, \theta, \lambda) = \iint d\theta d\lambda g_\lambda(\lambda) g_\theta(\theta) R_M \left(\theta - \frac{\lambda - \lambda_1}{\lambda_1} \tan \Theta_B \right) \cdot R_S \left(\omega + \theta - \frac{\lambda - \lambda_1}{\lambda_1} \tan \Theta_B \right) \cdot R_A \left(2\omega - \varepsilon + \theta - \frac{\lambda - \lambda_1}{\lambda_1} \tan \Theta_B \right) \quad (5)$$

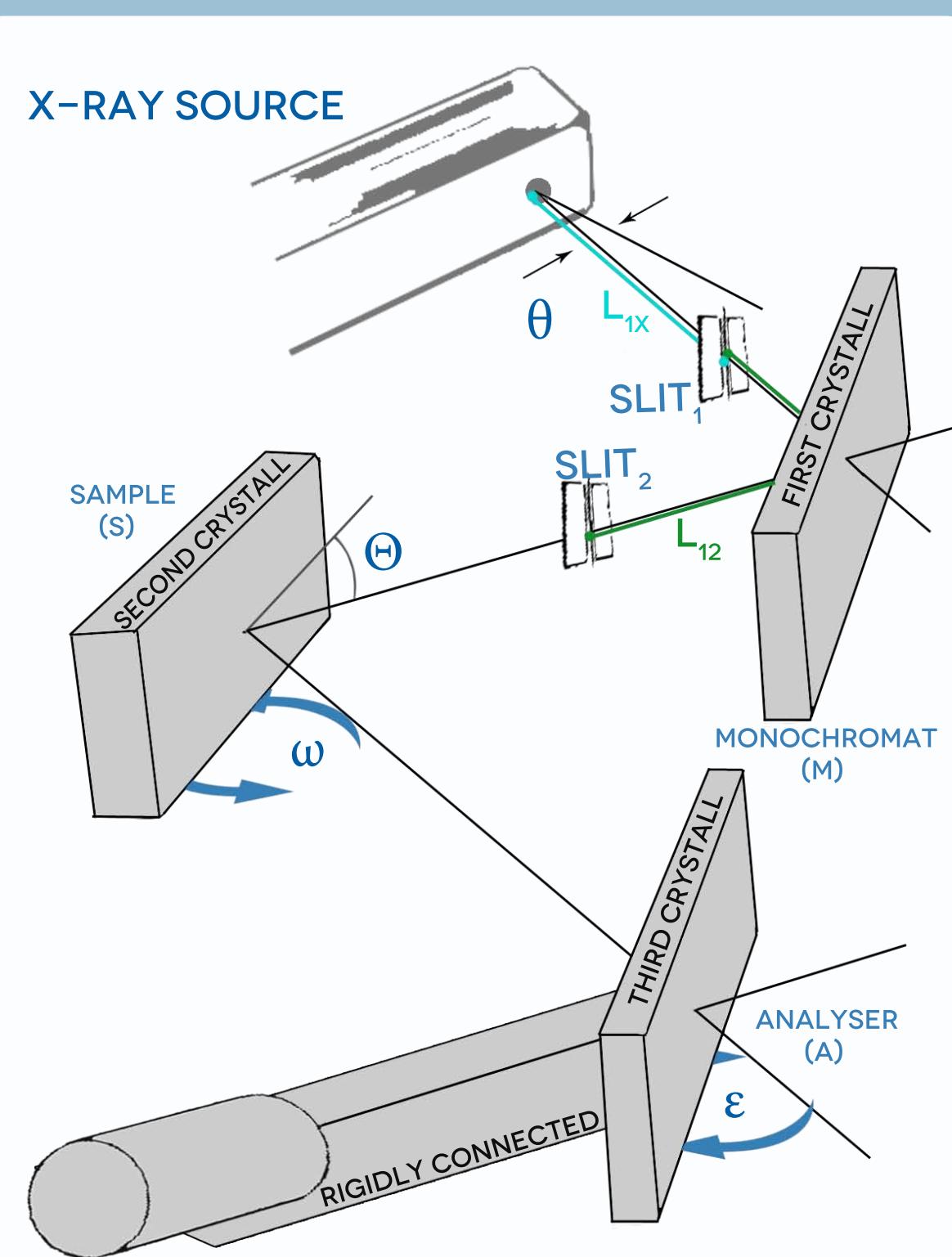
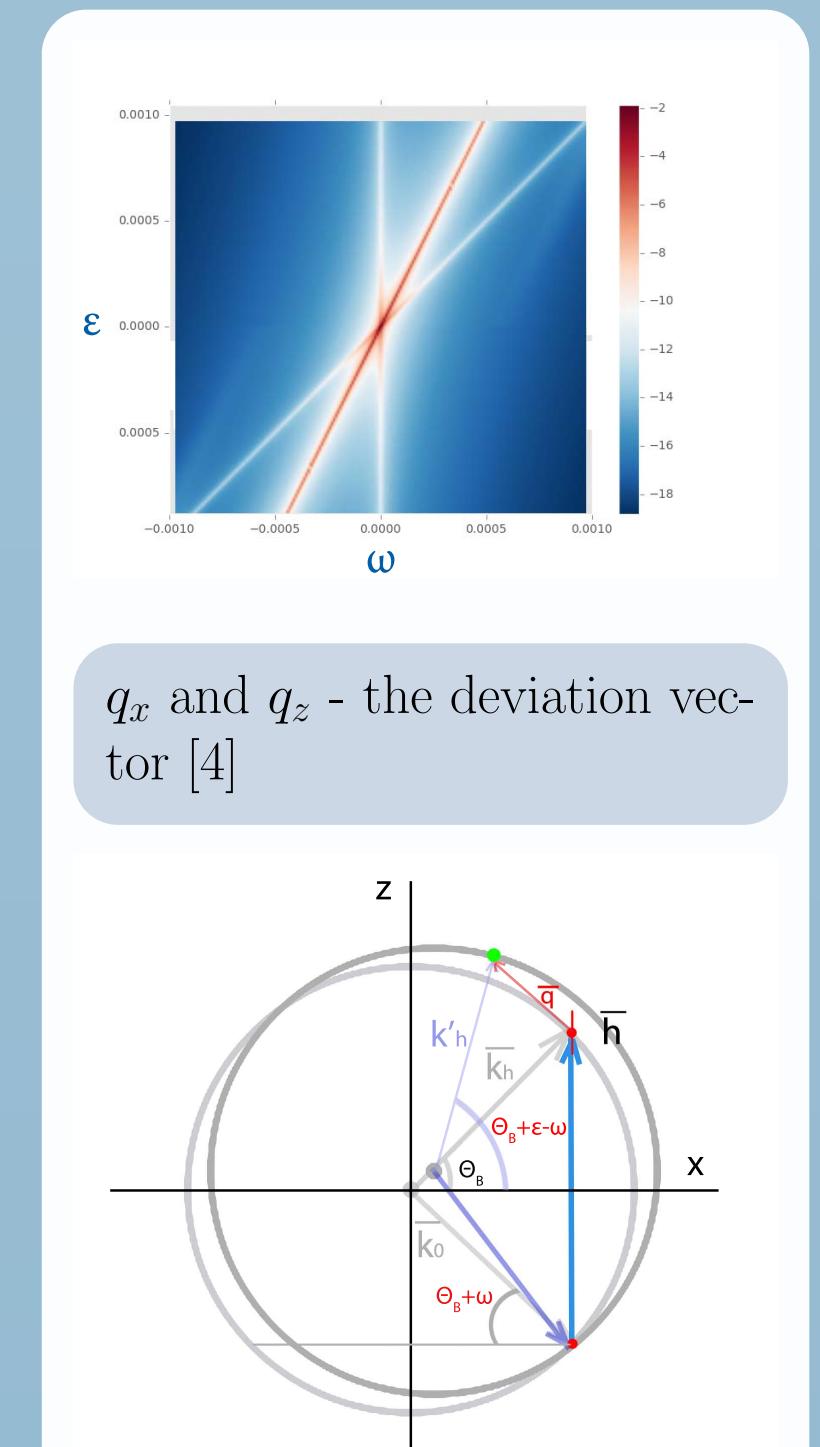


Figure 6: TCD experimental scheme

In the triple-axis mode, an analyzer crystal is placed after the specimen and before the detector. This is mounted on an axis concentric with the specimen and is scanned independently of the sample. The experimenter can then map the intensity distribution with respect to the direction of the radiation scattered by the specimen. This not only removes the complication of a possibly bent or mosaic specimen, but also enables one to distinguish scattering from various sources. For example, scattering due to defects occurs in a different direction in space from scattering from the perfect crystal and from a map of the scattering as both the specimen and analyzer are rotated, this can be measured quantitatively. Scattering from a rough surface can be separated from the perfect crystal scattering and most importantly, strain or mismatch may be distinguished from tilt or mosaic spread [4].



symmetrical case,

$$\begin{cases} q_x = (2\omega - \varepsilon) \cdot \sin(\theta_B) \\ q_z = \varepsilon \cdot \cos(\theta_B) \end{cases}$$

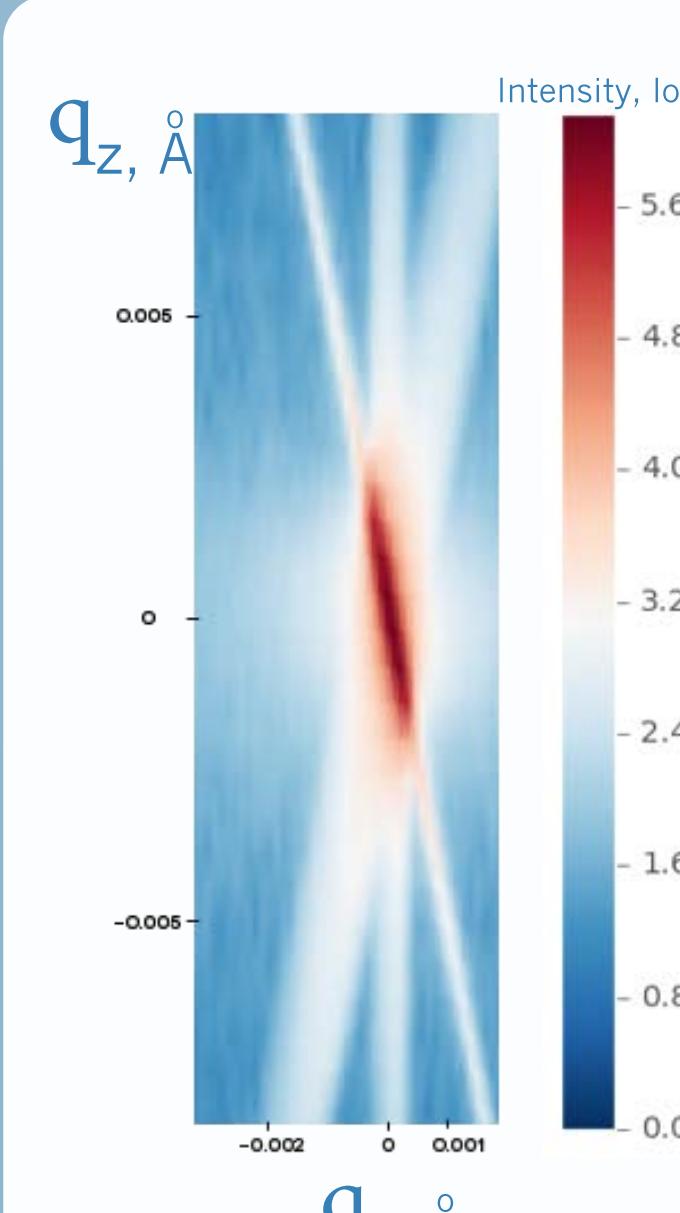


Figure 7: An experimental scattering map in reciprocal space.

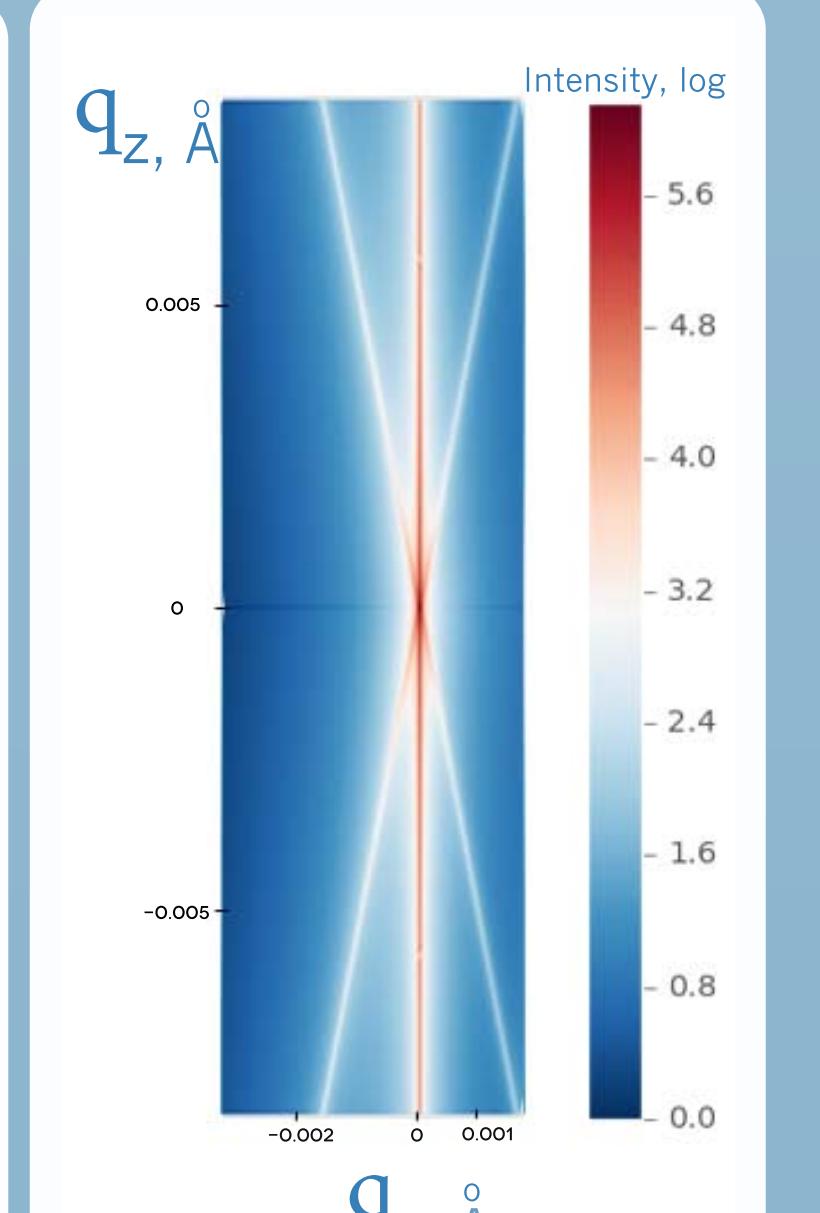


Figure 8: A simulated scattering map in reciprocal space.

References

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Conclusions

The results of experimental and theoretical analysis of the integral rocking curves in the non-dispersive (or not) X-ray double-crystal diffractometer schemes are discussed. It is shown that under certain conditions the secondary peak, which relates to the $MoK_{\alpha 2}$ -line of the incident X-ray characteristic radiation, takes place at the non-dispersive rocking curves. The trapezium and Monte-Carlo numerical methods are used for evaluations of the theoretical double- and triple-crystal rocking curves. Also, the attention is paid to triple-crystal refractometry. It involves the development of algorithms for reciprocal map calculations at the near of the exactly Bragg reflection. Here we create multithreaded application because of multitude calculus. At present the theoretical approach for diffusion calculations (statistical defects and thermal vibrations of atoms) is developing [5]. The computer program package is elaborated for the numerical calculations of the double- and multi-crystal rocking curves as the mathematical software for the X-ray diagnostics of real crystal structures by the double- and multi-crystal diffractometry methods.