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X-ray diffraction, defect structure, crystal diagnostics, x-ray diffraction under external influence, piezoelectric properties of crystals.

Development of the complex methods for numerical calculations of double- and multi-crystal rocking curves

The results of experimental and theoretical analysis of the integral rocking curves in the nondispersive 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 (Fig. 1). The trapezium and Monte-Carlo numerical methods are used for evaluations of the theoretical double-crystal rocking curves.

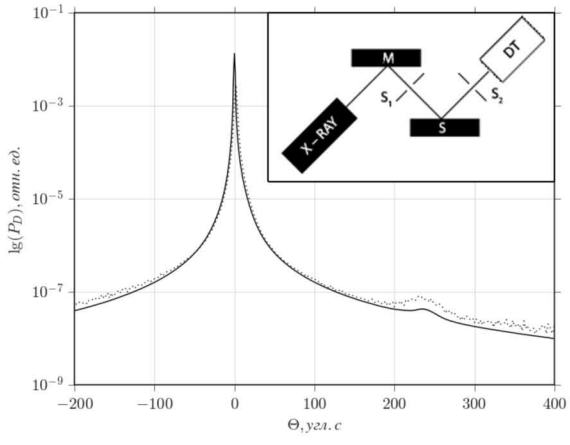

Fig. 1. Theoretical (solid) and experimental (dotted) non-dispersional rocking curves $P_{2D}(\vartheta)$: crystal-monochromator and sample are monocrystal Si, diffraction vector $\mathbf{h} = \langle 220 \rangle$, Bragg's angle $\theta_B = 10.64°$.

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.

[1] M.A. Chuev *et al.,* Crystallography Reports. 734-747 (2008) **53**.
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[3] P.V Petrashen, Metallofizika. 35-43 (1986) **8**.
[4] P.V. Petrashen, F.N. Chukhovskii , Metallofizika. 45-51 (1986) **8**.