The results of experimental and theoretical analysis of the rocking curves in double- and triple-axis X-Ray diffraction schemes are discussed. New calculation algorithm is developed which takes into account a diffractometer instrumental functions such as spectral functions of synchrotron or laboratory sources and angular divergence function, determining by size of collimators (slits) and optical lengths between optical elements of experimental facility. Rocking curve calculations for the general dispersive case including asymmetric reflections are given. It is shown that under certain conditions the secondary peak, which relates to the line of the incident X-ray characteristic radiation for laboratory source takes place at the rocking curves [2].

The results of 2D reciprocal space map calculation in the area of reciprocal lattice node for the Si crystal corresponding to those obtained by the triple-axis X-Ray diffractometry technique are presented. There is developed theoretical approach to describe general pattern of X-Ray scattering including diffuse scattering for real crystals. It is based on model proposed in [3], in which the basis of physical processes of diffuse X-Ray scattering was suggested. In the case under consideration, defects of crystal structure are statistically distributed and the average concentration is a function of depth from surface inside a crystal.

In order to decrease the time spent on calculations the Monte-Carlo numerical methods, multi-threading calculation and supercomputer are used.

The computer program package is elaborated for the numerical calculations of X-Ray rocking curves as the mathematical software for the X-ray diagnostics of real crystal structures by the double- and triple-axis X-Ray diffraction methods.