Verification of a New X-ray n-Beam Dynamical Theory using an Arbitrary-polarization-generating X-ray Phase-retarder System

While an ordinal diffraction case in which the incident X-ray beam and only one reflected X-ray beam are strong in the crystal is called the two-beam case, cases in which more than one Bragg-reflected X-ray beams are strong are called n-beam cases when n beams are strong.

The present author has, for the first time, derived a Takagi-Taupin-type X-ray n-beam dynamical theory [1,2] which can deal with X-ray n-beam wave fields in a distorted crystal without neglecting the polarization effect. The new theory has a simple form that can be written by one partial differential equation supposing that suffixes are taken in $2n$ ways.

On the other hand, the present author and co-authors have developed a rotating four-quadrant phase-retarder system to generate arbitrarily polarized X-rays from the horizontally polarized synchrotron radiation based on the four-quadrant phase-retarder system [3]. Because the behavior of X-ray n-beam wave fields excited in a crystal is expected to strongly depend on the polarization state of the incident X-rays, the apparatus for generating arbitrarily polarized X-rays will have an effective role in experimentally verifying the new n-beam dynamical diffraction theory.

Figure 1 shows the rotating four-quadrant phase-retarder system for generating arbitrarily polarized X-rays. Four diamond crystals with a total thickness of about 8 mm were set on small tangential-bar goniometers in a χ-circle goniometer with an angular interval of 90 deg. The angular deviations of diamond crystals from the Bragg conditions of 1 1 1 reflection in an asymmetric Laue geometry and the rotation angle of the χ-circle were controlled properly to generate the objective polarization states of X-rays (18.245 keV; the Bragg angle of 0 8 8 reflection is almost 45 deg and free from the glitch of diamond crystals used for phase retarders). Figure 2 shows a schematic drawing around the sample FZ silicon crystal of 9.6 mm thickness arranged to take six-beam 'pinhole topographs' [2,4] with the incidence of X-rays whose polarization state was controlled. After the orientation of the sample silicon crystal was adjusted by monitoring forward-diffracted, 4 4 0-reflected and 4 8 4-reflected X-rays to satisfy the six-beam condition, the dimensions of X-ray beams were limited to a width of 25 μm and a height of 25 μm. Six-beam topograph images were simultaneously recorded on an imaging plate with a pixel size of 50 μm square placed about 27 mm behind the sample crystal. The *Experimental* topograph images of 0 0 0-, 4 4 0-, 4 8 4- and 0 8 8-reflected X-rays with an incidence of *left*-circular polarization are shown in the left column of Fig. 3 together with the corresponding computer-*Simulated* topographs based on the new theory in the right column. Also with the incidence of other polarization states, experimental and simulated results agreed well, while their evident differences were found to be strongly dependent on the polarization states of the incident X-rays. Thus, the applicability of the new n-beam X-ray dynamical theory and the efficiency of the rotating four-quadrant phase-retarder system were simultaneously confirmed.

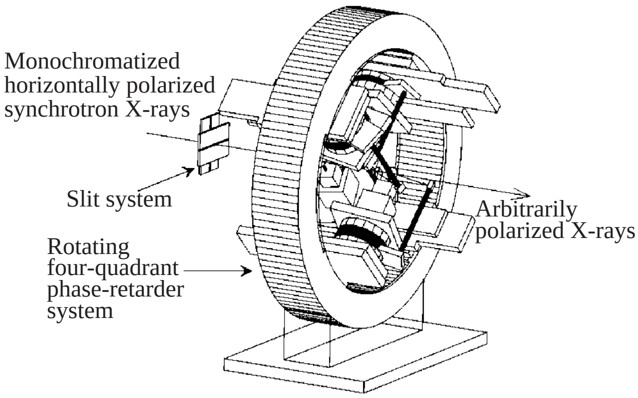

Fig. 1. Rotating four-quadrant phase-retarder system.

Incidentally, there is a big problem in the crystal structure analysis, that is, the phase values of crystal structure factors cannot be obtained with ordinal (two-beam) X-ray diffraction experiments (phase problem). It has been known from many years ago (1930s) that the phase information of crystal structure factors can be extracted from X-ray intensity profiles in the vicinity of the n-beam condition. This is a dynamical diffraction effect. However, most of the crystals whose structures have to be solved exhibit marked distortion, thus the conventional n-beam (limited to three-beam) dynamical theory cannot be directly applied to such crystals. In almost all cases of crystal structure analysis, the kinematical diffraction theory has been applied.

The final purpose of the present study is to construct an n-beam dynamical theory applicable to

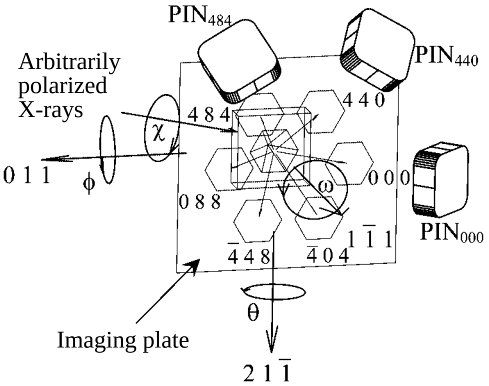

Fig. 2. Schematic drawing around the 111-oriented FZ silicon sample crystal [2].

solving the phase problem of large molecular crystals. In 1970s-1980s, Kato constructed the statistical dynamical theory based on Takagi-Taupin equations, which deals with lattice displacements in a distorted crystal statistically and describes X-ray wave fields in mosaic crystals. Therefore, a new *n*-beam dynamical theory that describes X-ray wave fields in mosaic crystals and extracts the phase information will be constructed using Kato's statistical procedure for lattice displacements based on the theory derived by the present author [1,2].

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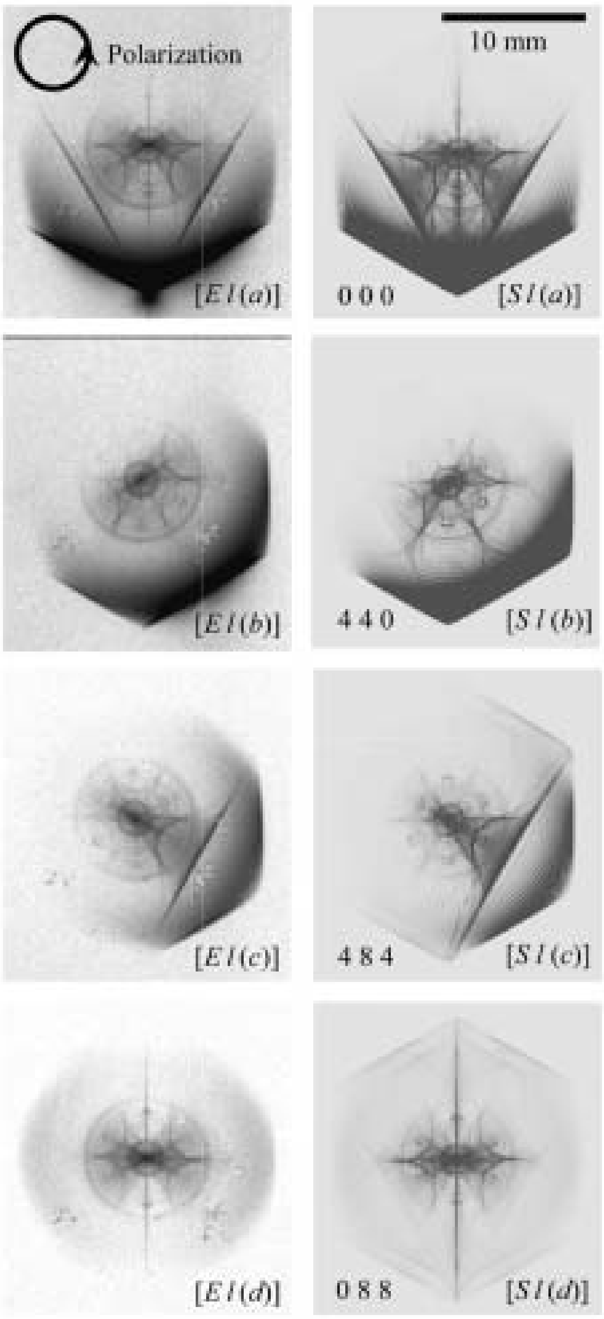

Fig. 3. Left and right column figures show *Experimental* and computer-*Simulated* pinhole topographs with the incidence of *left*-screwed circular polarization. (*a*), (*b*), (*c*) and (*d*) correspond to 0 0 0-, 4 4 0-, 4 8 4- and 0 8 8-reflected X-ray images, respectively [2].