BL02B1
Single Crystal Structure Analysis

1. Introduction

BL02B1 is designed for single-crystal structure analyses and is equipped with a two-dimensional (2D) hybrid pixel detector, PILATUS3 X CdTe 1M (Dectris). The silicon double-crystal monochromator can select monochromatic X-rays between 8 keV and 115 keV from synchrotron X-ray radiations of the bending magnet. Most of the current experiments use monochromatic X-rays between 18 keV and 60 keV. BL02B1 currently promotes charge density studies and *in situ* experiments for functional materials using the PILATUS3 X CdTe 1M detector. The 2D detector with CdTe modules is very useful for detecting high-energy X-rays because of their high efficiency. To use high-energy X-rays, crystal structure analysis can be performed for inorganic materials with heavy atoms. Because the PILATUS3 X CdTe 1M provides statistically accurate data due to the wide dynamic range, it is used for precise structure analyses, especially in charge density studies.

2. Development of a new control program for single-crystal X-ray diffraction measurement

In FY2021, we continued developing a fully automated measurement project for the single-crystal structure analysis of small molecules. This project aims to load the mounted sample into the sample magazine, start the measurement, and obtain the data needed for single-crystal structure analysis. In FY2020, we developed the automatic centering program, which moves a crystal sample to the center of the goniometer. For fully automated measurement, measurement software is necessary, which can work with the automatic centering program. However, it is difficult to add these functions to the current program for controlling diffractometers. On the basis of this, in FY2021, we developed a program for the single-crystal X-ray diffraction measurement using Python3 (Fig. 1). This new software can control the diffractometer and the detector and generate the files necessary for single-crystal structure analysis. Additionally, the
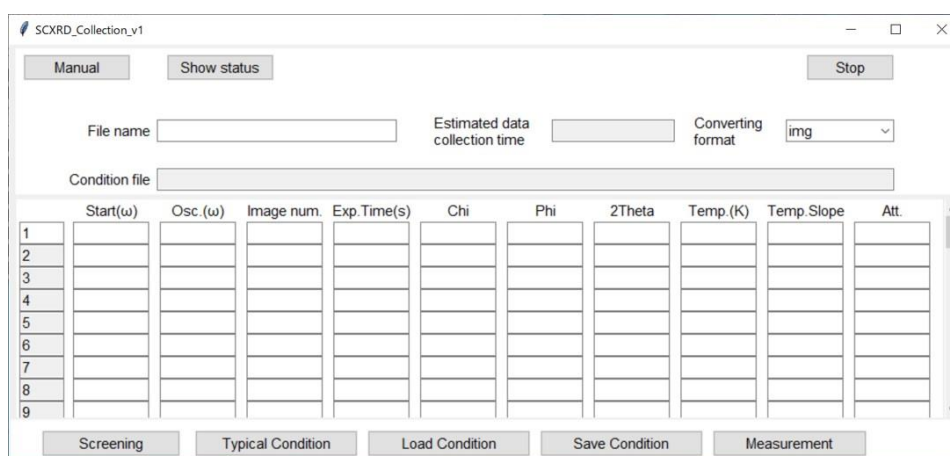

Fig. 1. New control program for single-crystal X-ray diffraction measurement.

program implements software limit functions not previously included, eliminating the possibility of instrument errors due to the incorrect input of experimental conditions and improving safety. The function of this program is to send commands to the old controller for the diffractometer. However, we plan to replace the old controller for the diffractometer with more stable and faster pulse motor controllers and motor drivers.

In summary, a fully automated high-throughput single-crystal structure analysis measurement system is under development. We plan to construct a fully automated measurement system in which the user only needs to specify the sample ID numbers to be measured to complete the series of measurements.

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