BL02B1
Single Crystal Structure Analysis

1. Introduction

BL02B1 at SPring-8 is dedicated to high-energy single-crystal X-ray diffraction and is equipped with a versatile four-axis diffractometer (2θ, ω, χ, φ) combined with a two-dimensional hybrid pixel detector, the PILATUS3 X CdTe 1M (DECTRIS AG). Monochromatic X-rays in the 18–60 keV range are provided by a Si(311) double-crystal monochromator, optimized for the bending-magnet source. The CdTe sensor of the PILATUS3 detector offers outstanding efficiency for hard X-rays together with a very wide dynamic range, ensuring precise intensity measurements even in the presence of heavy atoms. These features make the beamline especially powerful for challenging experiments such as charge-density determinations, the detection of subtle structural distortions, and a wide range of in-situ studies. To take full advantage of these experimental capabilities, the continuous development of advanced data processing and automation tools is essential.

1. Implementation of open-source program DIALS for data analysis

In FY2024, we implemented the open-source program DIALS for data analysis. Commercial software like CrysAlisPro or APEX, while widely used, suffers from opaque algorithms, limited customization, and GUI-bound workflows that hinder advanced or automated studies. To overcome these limitations, we introduced the open-source DIALS framework at BL02B1 [1]. Its transparent, modular design enables fine-sliced data to be processed flexibly and integrated seamlessly into automation. A Python-based converter was developed to transform .tif images into DIALS-compatible full .cbf files, making full processing within DIALS possible. Initial tests on the standard FeV_2O_4 compound produced results in excellent agreement with those obtained using commercial software, establishing DIALS as a reliable and automation-ready solution for BL02B1.

2. Development of automated data analysis pipeline AUDI (Automated DIALS)

To achieve full automation in data processing at BL02B1, we have developed AUDI, a Python-based pipeline built on DIALS, as shown in Fig. 1. AUDI, now available in GUI format, as shown in Fig. 2, converts raw images to full .cbf format, performs

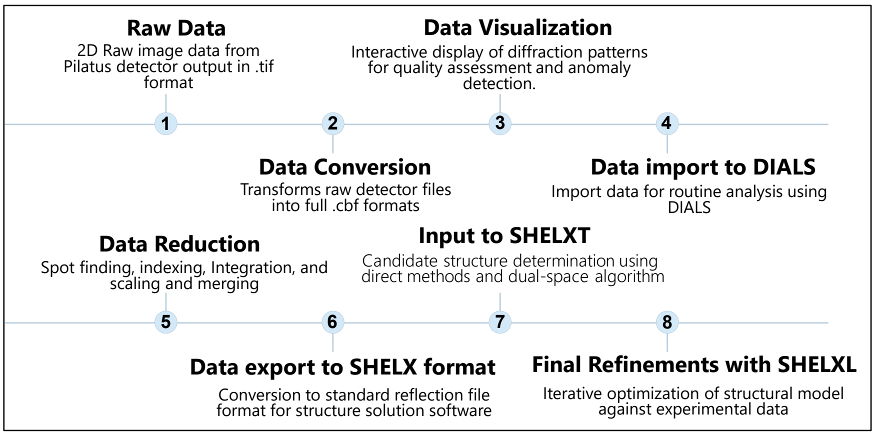

Fig. 1. AUDI automated workflow, showing the sequence from raw diffraction images through data processing to final structure candidates.

indexing, integration, scaling, and merging, and proceeds through structure solution with SHELXT and routine refinement using SHELXL with minimal user input. An interactive viewer allows a quick inspection of the data frames, and the result section highlights key metrics and candidate structures. The system can run in parallel with data collection, reducing the total processing time from hours (or even one day for ultrafine sliced data) to minutes. Designed for transparency and extensibility, AUDI avoids "black box" limitations of commercial programs and is readily adaptable for advanced charge density analyses. Importantly, it not only supports experienced users but also enables novice users to complete high-quality analyses independently and obtain results that are close to being final already during beamtime.

3. Extension of AUDI for automated charge density analysis through CDFS and MEM

As a future direction, we are working to extend AUDI to automate advanced charge-density studies by integrating workflows for core differential Fourier synthesis (CDFS) and the maximum entropy method [2,3] (MEM). This will allow direct transition from raw diffraction images to electron-density reconstruction with minimal user intervention. Such an extension will enable a near real-time evaluation of bonding and electronic structure during beamtime, establishing BL02B1 as a unique platform for automated charge-density research.

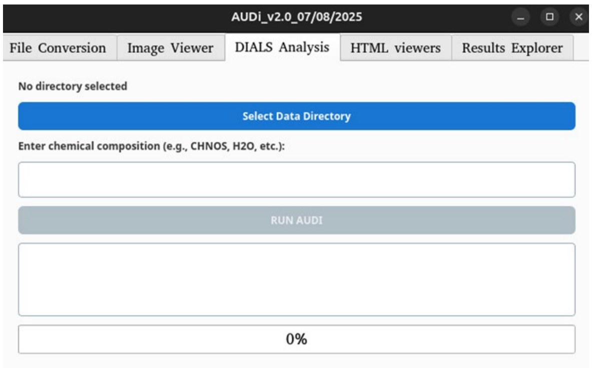

Fig. 2. AUDI graphical user interface (GUI) with multiple tabs for visualization, structure solution, and real-time result inspection.

Together, the implementation of DIALS, the development of AUDI, and its planned extension toward automated charge-density analysis represent a major step in advancing data processing at BL02B1. These tools not only improve efficiency and reliability for complex experiments but also broaden accessibility, allowing both experienced and new users to achieve high-quality, publication-ready results. By combining precision, automation, and transparency, BL02B1 is positioned to remain at the forefront of precision structure analysis at the charge density level and to support cutting-edge research on functional materials.

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