Engineering and implementation of the new diffractometer – D3 – for the macromolecular crystallography beamlines of the Swiss Light Source

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Abstract. For the three macromolecular crystallography beamlines of the Swiss Light Source, a new unified diffractometer - D3 - was developed. We present details of the engineering and implementation of the project components that were fabricated in-house by the design facilities of the Paul Scherrer Institute (PSI). Key components of the diffractometer project were custom designed at PSI including a microspectrophotometer for sample viewing and optical spectroscopy and a combined Köhler and spectroscopic illumination lamp. In addition, all elements for beam steering and shaping such as an exposure box and multiple articulated elements for beam shaping and beam diagnostics were designed in-house. Further components are the positioners for cryo-cooling devices, and an X-ray-fluorescence detector. For minimization of vibrations, a combined mineral cast and granite block design was employed for the diffractometer table. Due to the restricted space of the sample environment, a high degree of integration of the D3 instrumentation had to be achieved. Devices to be considered in the integration concept are the robotic sample changer, the area detector and the new multi-axis goniometer PRIGo. Optimization strategies include kinematic simulations to describe the kinematic hull structure of the sample positioning and to reduce possible collisions. Additionally, flexure designs were used to allow adjustability while satisfying space constraints.

1. The project and its components

The new unified D3 diffractometer for the macromolecular crystallography beamlines of the Swiss Light Source comprises an on-axis microspectrophotometer for sample viewing and optical spectroscopy, beam steering and shaping elements, beam diagnostics, a cryo-cooling device, an X-ray fluorescence detector and an Irelec robotic sample changer (CATS) [1]. In addition to the integration of the Köhler illumination of the new on-axis microscope, the PRIGo multi axes goniometer [2] and the X-ray diagnostics instrumentation, the goal to reduce the distance between the Dectris Pilatus 6M detector [3] and the specimen from 165 mm to 120 mm could be fulfilled.

The successful integration was, among others, attributable to the kinematic simulations, the customised optical design, the use of flexure based adjustments for space constrained applications and the use of rapid prototyping to quickly and economically realize elaborate enclosures largely constrained
by the confined spaces. The following sections describe the details of the engineering and implementation process.

The first unit was installed at beamline X10SA during the April 2012 shutdown. Two more units with modifications tailored to the particulars of the beamlines will be installed at beamlines X06SA and X06DA.

![Figure 1. The new unified D3 diffractometer and a detail of the sample environment.](image)

2. **Kinematic simulations**

The tight space constraints, e.g. the microscope objective's 34 mm and the illumination objective's 15 mm working distance, are limiting the mobility of the PRIGo multi axis goniometer, depending on the goniometer state (angles and translations) and the diffractometer operational state.

![Figure 2. The multi axis goniometer and its envelopes for different chi angles (0° in the left figure and 45° in the right). The limitations in accessible parameter space are visible. The envelopes were used to optimise the design and the overall flexibility of the instrument concurring with the PRIGo goniometer with an iterative approach.](image)
Because of the space constraints it was necessary to perform kinematic simulations to detect possible collisions early in the process of development. Hence, a set of envelopes of the PRIGo for different sample pin tilt angles (\(\chi\)) were calculated and used to predict the final mobility of the multi axes goniometer for the different diffractometer states and for different lengths of sample pins. The envelopes were used to optimize the design and the overall flexibility of a final version of the instrument currently in development. Until final commissioning of this device, a single axis goniometer is used.

3. Beam shaping and diagnostic unit - flexure designs

The beam shaping and diagnostic unit contains an aperture-assembly for beam size control, a collimator for stray light reduction and a scintillator / diode combination for diagnostics. Apertures with diameters of 150, 30 and 10 \(\mu\)m are in use. For each of the instrumentation fingers, a flexure design was used not only to allow for adjustability and to meet precision requirements, but also to cope with the limited space constraints. The target resolution of 0.5 \(\mu\)m and also the repeatability of the movers below 1 \(\mu\)m could be met using flexure hinges.

The magnetic kinematic mounting base allows the manual removal of the beam conditioning elements while ensuring a reproducible remounting.

![Figure 3](image)

**Figure 3.** (a) The beam shaping and diagnostic unit is illustrated on the left. On the right (b) the manual flexure adjustment assembly and (c) the magnetic kinematic mounting are shown.

4. Optical table

Minimizing the vibrations of the table and the instrumentation is relevant for the operation of the diffractometer. The D3 solution is closely related to the SwissFEL undulator girders [4]. A stable composite structure was used for the table design. It consists of a welded steel shell and cast structure filled with an epoxy resin-bonded mineral casting material. Its total weight is about 2 tons. For adjustment of the table position, three SwissFEL girder feet are used. The amplification ratio of the RMS displacement from table to floor is below 2.0 (5 to 200 Hz).

A granite block design was chosen to increase the flexibility of the main instrumentation components on the table, without compromising on the stiffness and damping of the supports.
5. Rapid prototyping
The rapid prototyping method was used to fabricate cost effective and quick realization of enclosures with complex shapes. The technique was used for covers and small lids used to protect the delicate components on top of the beam shaping and diagnostic unit and its instrumentation fingers. This enables safe manual manipulation by the synchrotron staff and users during setup and manual sample exchanges between measurements.

6. Optics
The newly developed microspectrophotometer is in full user operation for sample viewing, with an image resolution of 1 micron and a minimum field of view of 0.5 x 0.38 mm. First commissioning measurements with the absorption and the Raman spectroscopic operation modes have successfully been performed. The data and the detailed optical design will be published in a separate paper.

![Figure 4.](image)

Figure 4. (a) The microspectrophotometer “MS3” and its components. (b) Both light paths – for the microscopic and the spectroscopic branches are illustrated. (c) The MS3 spectroscopic branch with its optical components.

A custom modular design was chosen for the body of the microspectrophotometer. It features a fixed high magnification and a fixed low magnification optical microscope, as well as a separate spectroscopic branch. A custom flip beam splitter to couple the spectroscopic branches was developed due to the space constraints. Standard optical components have been used where possible. To enable flexible spectroscopic analysis, a removable cube design was employed to rapidly switch between the absorption, fluorescence and Raman measurement modes. The combined Köhler and spectroscopic illumination unit is fully retractable to avoid the shadowing of the detector during diffraction operation.

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8. References
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