

Development of automated home-lab beamlines

Vernon Russell Smith¹, Matthew Benning², Joerg Kaercher², Matthias Binkele¹, Jaap Toorn¹
¹Bruker AXS, Karlsruhe, Germany, ²Bruker AXS, Madison, United States
E-mail: vernon.smith@bruker.com

For over a decade high flux synchrotron beamlines have focused intensely on automating their macromolecular crystallography beamlines in to increase throughput, reduce sample handling errors and improve data quality. This focus has been driven by the fact that highly intense beams coupled with fast detectors now enable complete data sets to be collected in only minutes. As a result the deadtime attributed to sample mounting and centering consumed the vast majority of the total experiment time. The pressure to mount and center crystals quickly rapidly increased the number of samples lost due to handling errors.

Bruker AXS integrated the ultra-high brilliance METALJET source into their D8 VENTURE platform over five years ago, and subsequently developed the first CPAD detector designed specifically for compatibility with such X-ray sources. Users of such a in-house beamline have found that they face similar difficulties to those experienced at synchrotron beamlines before modern automation was introduced.

Here, we will introduce new developments made by Bruker AXS in automating their high-brilliance D8 VENTURE systems, namely SCOUT, AGH and ISX STAGE.

The SCOUT Automated Sample Changer is a six-axis robotic system designed for the automated sample mounting, centering and retrieval of crystal under cryogenic conditions. Unlike earlier such robots, SCOUT has been conceived and designed specifically to meet the demands of in-house crystallography. The priority has been on maximizing the reliability of sample mounting and retrieval, and minimizing iceing. This ability to retrieve crystals and return them to storage in LNW without ice accumulation is an area that is much more demanding than in synchrotron crystallography, where crystals are typically discarded after exposure. An advanced software GUI enables automated crystal centering, scoring and data collection.

The AUTOMATED GONIOMETER HEAD is a highly robust goniometer head designed for fast crystal centering in combination with a KAPPA goniometer. In addition to optical crystal centering, the AGH features, for the first time in-house, the ability to center crystals using their X-ray diffraction. This enables much more accurate centering of small crystals by eliminating parallax errors associated with optical centering. It also enables the reliable centering of crystals embedded in opaque LCP. the ability to center on the "diffraction hotspots" of larger crystals provides a further route to obtaining the best quality data from the crystals available.

The ISX STAGE is the only automated plate-stage compatible with a KAPPA goniometer. The methods development associated with room temperature in situ crystallography over recent years have been mirrored in the popularity of the ISX STAGE. Here, we will review the key features of the stage and highlight the key applications.

Keywords: [x-ray centering](#), [automation](#), [in situ](#)