

Automation at the Automated Macromolecular Crystallography (AMX) beamline at NSLS-II

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The Automated Macromolecular Crystallography (AMX) beamline is a microfocus MX beamline located at the National Synchrotron Light Source-II (NSLS-II), Brookhaven National Laboratory (Upton, NY USA). The X-ray beam at AMX is focused to a fixed size of a 7x5 μm with a flux of approximately $4.1\text{E}12$ ph/s at 475 eV. Focusing is accomplished with tandem vertical and horizontal Kirkpatrick Baez mirrors situated approximately 2.68 m and 1.97 m respectively from the sample position. These features make AMX well-suited for measuring challenging samples that include microcrystals; crystals with large unit cells; and clusters of crystals that display multiple lattices. The main collection modes at AMX are raster scans, standard collections, and vector collections (rotation combined with translation parallel to the horizontal rotation axis). Optimal sample centering is achieved at AMX with multiple raster scans collected at orthogonal sample orientations. In the automated collection mode a collection rate of approximately 320 samples/day can be achieved with automated raster scanning or 500 samples/day with optical loop centering. Since user operations began in 2017 approximately 53,000 raster scans have been collected at AMX in addition to 28,000 standard collections and 11,000 vector collections. The microbeam at AMX creates many challenges and opportunities for automated data collection. In-line processing of raster scans is achieved with a fast spotfinder and local compute cluster. New algorithms for the optimal handling of multi-lattice data, sample centering with computer/machine vision, and automated decision making are all currently under development and will be discussed in this presentation.