

Automated Crystal Diffraction Screening Hardware: Component V (headed by Thomas Earnest) has implemented hardware and beamline control software at the Advanced Light Source beamlines (5.0.1, 5.0.2 and 5.0.3) for automated crystal screening. These components are used in combination with the automated data analysis tools developed by the center to automatically screen crystals.

Robotic Hardware: The beamlines currently available to the Center each have a robotic crystal mounting system, developed under NIH R01 funding to Thomas Earnest. The robot has a large liquid nitrogen dewar and cryo-pin gripper assembly (Fig. 1). The dewar is rotated and translated in order to position the required crystal under the gripper assembly. The gripper is then translated vertically out of the dewar, rotated by 90 degrees, and is translated horizontally to place the cryo-pin on the goniometer. Crystals are mounted on cryo-pins and placed in circular “pucks” that are able to hold 16 samples (Fig. 1). Up to 7 of these pucks can be accommodated in the robot dewar. The pucks have been designed to fit in a standard shipping dewar. The robotic system has been experimentally tested to show that diffraction quality is not affected by its use (Snell et al., 2004). In addition, the robot is routinely used by other researchers. Once a cryo-pin is placed on the goniometer, the loop is auto-centered using optical image analysis routines. The beamline software also provides the capability to manually center the crystal using a point-and-click user interface. A screening interface allows the user to select which crystals in the robot dewar are to be screened. Once the start button is activated, the crystal mounting, loop centering, image collection, and diffraction analysis are performed automatically for each selected crystal. As analysis results are generated, they appear in the screening interface in real-time. To assess the quality of each crystal, two diffraction images are collected. These images are then analyzed using the LABELIT software (Sauter, Grosse-Kunstleve & Adams, 2004). The development of the automated crystal screening system has made it possible to automatically screen up to 112 crystals without the need to enter the experimental hutch.

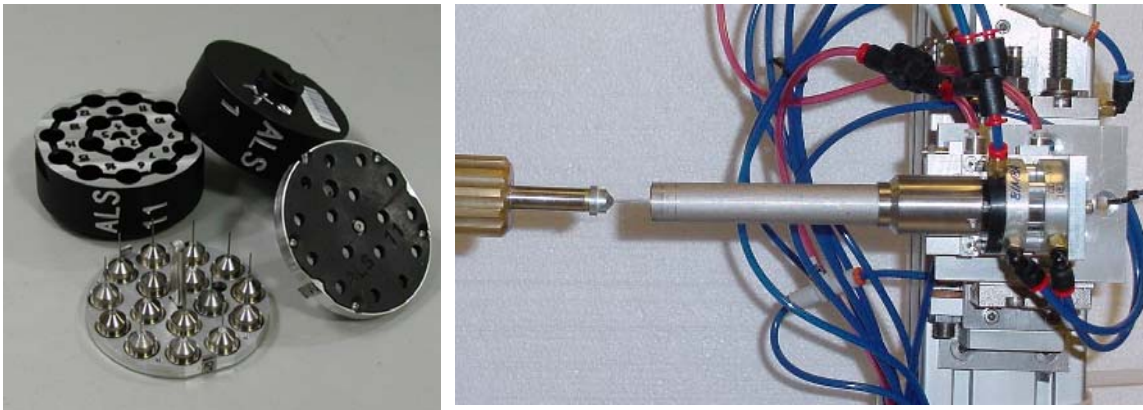


Fig. 1. Left, automounter puck containing 16 crystals. Right, close-up of the automated robot crystal gripper arm.