X-Ray Diffraction Systems

The Materials Characterization Center (MCC) has two independent X-ray diffractometers (Figure 1) enabling the study of polycrystalline and single-crystal samples with long range order in all three dimensions with the d-spacing up to ~1 nm.

Figure 1: Siemens/Bruker D5005 X-ray diffractometer (left) and Siemens/Bruker GADDS X-ray diffractometer (right).

Siemens/Bruker D5005 X-ray Diffractometer

A fully automated Siemens/Bruker D5005 Theta/2 Theta Bragg-Brentano diffractometer is configured for high-precision crystallographic investigations of polycrystalline samples. This diffractometer is equipped with 2.2 kW sealed Cu X-ray source, high-precision vertical Theta/2 Theta goniometer, standard sample stage, curved graphite crystal diffracted beam monochromator, and NaI(Tl) scintillation counter detector. X-ray powder diffraction applications for this instrument at MCC include qualitative and quantitative phase analysis, crystallite size and lattice strain measurements, precise lattice parameter determinations, line profile shape analysis, and structure refinement by the Rietveld method. The instrument is fully supported by complete data reduction and analysis software.

D5005 Specifications

2.2 kW FL Cu 4KE type air-insulated X-ray diffraction tube with Cu anode.
Standard sample stage (no sample rotation, no automatic changeover of multiple samples).
Reflection measurements only.
**Siemens/Bruker General Area Detector Diffraction System (GADDS)**

A General Area Detector Diffraction System (GADDS) with HI-STAR area detector and PLATFORM goniometer allows high speed and sensitivity of data collection and is configured for crystallographic investigations of polycrystalline or single-crystal samples, and examinations of small sample quantities with very high counting and particle statistics. This diffractometer is equipped with 2.2 kW sealed Cu X-ray source, flat graphite crystal monochromator, various collimators, beam stop, high-precision horizontal PLATFORM Theta/2 Theta goniometer, fixed-chi sample stage, optical microscope for sample alignment, and HI-STAR two-dimensional detector. Applications for this instrument at MCC include rapid phase identification, degree of crystallinity determinations, characterization of preferred orientation and texture, and crystal quality determination. The instrument is fully supported by complete data reduction and analysis software.

**GADDS Specifications**

- 2.2 kW FL Cu 4KE type air-insulated X-ray diffraction tube with Cu anode.
- Samples can be mounted in transmission or reflection mode.
- Powders can be mounted in glass capillary.
- Small and medium samples can be analyzed on a flat plate.
- Detector-to-sample distance = 6-30 cm.
- Collimators are 0.8, 0.5, 0.3, and 0.2 mm in diameter.