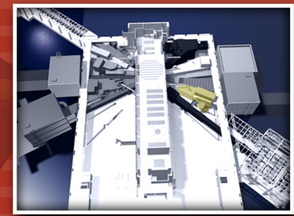
Instrument Fact Sheet

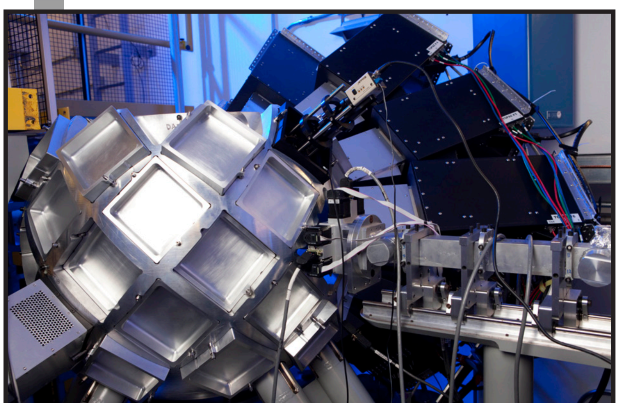
BEAM LINE 12

SPALLATION NEUTRON SOURCE



TOPAZ – Single-Crystal Diffractometer

TOPAZ can address problems in chemistry, earth sciences, materials science and engineering, solid-state physics, and biology. A wavelength resolved (= time-of-flight) Laue neutron single-crystal diffractometer with extensive area detector coverage, it is well suited for three-dimensional reciprocal or Q-space mapping of Bragg peaks and magnetic and diffuse scattering patterns from a stationary crystal at multiple setting angles. Experiments can be conducted in ambient conditions or in controlled sample environments. A nitrogen cold stream provides temperature control in the range of 100 to 450 K to collect data as a function of temperature. Two tunable neutron wavelength bands are available for data collection: magnetic and nuclear scattering are collected simultaneously. Moreover, the sample can be oriented with high precision to collect magnetic peaks in specific directions. Currently, 11 of 48 detector locations are populated with Anger camera modules covering a scattering angle of about 16–158° 2θ, matching 1.4 sr in an almost spherical arrangement around the sample. A full dataset for structure analysis can be collected in 15–30 settings, depending on crystal symmetry, with a minimum exposure time of about 15 minutes each, depending on scattering strength and sample size



Applications

TOPAZ is well suited for determining atomic positions and displacement parameters of light elements (such as hydrogen) next to heavy metals and for the study of magnetic structures, phase transitions, disorder, and local structure phenomena. Examples span a wide range of materials:

- Functional inorganic materials for the study of the interplay of nuclear and magnetic structure and spin arrangements such as magnetic superstructures in perovskites and spinels and single-molecule magnet materials.
- Hydrogen storage and other porous framework materials for the study of the guest-host interaction and guest mobility such as in metal organic framework materials and zeolites.
- Catalytic and dihydrogen activation or exchange materials for the study of metal-hydrogen bonding such as for catalytic precursors, metal-hydrides, and organometallics.
- Expansive organic molecules for the study of the hydrogen network, interaction at the active site or cavity, such as for enzymes and supramolecules.

Specifications

Moderator	Decoupled poisoned hydrogen
Source-to-sample distance	18 m
Sample-to-detector distance	39–45 cm
Angular detector coverage	1.7 sr (14 detectors)
Detector pixel size	1 mm
Detector angles	20–160°
Wavelength bandwidth	3.0 Å
Accessible wave length	0.5–3.5 Å
Frame 1	0.5–3.5 Å
Resolution	~0.4
Sample size	1 mm^3 < S < 10 mm^3
Neutron beam divergence on sample	15 mrad < d < 25 mrad

Status: In commissioning

For more information, contact

Instrument Scientist: Christina Hoffmann, hoffmanncm@ornl.gov, 865.576.5127
Instrument Scientist: Xiaoping Wang, wangx@ornl.gov, 865.200.2500

neutrons.ornl.gov/topaz

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