Spallation Neutron Source

BEAMLINE
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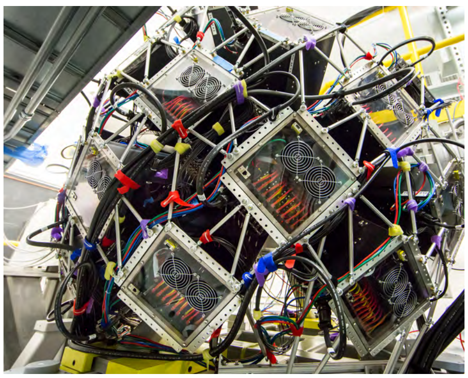
TOPAZ

Single-Crystal Diffractometer

TOPAZ is a high-resolution single-crystal diffractometer using wavelength-resolved Laue technique with an extensive array of neutron time-of-flight area detectors to address structural problems in diverse research areas: chemistry, earth sciences, materials science, engineering, and solid-state physics. Experiments can be conducted in ambient conditions or controlled sample environments for parametric study (temperature and electric field). A nitrogen cold stream offers temperature control in the range of 90 K to 450 K or a cryogenic goniometer equipped with a pulsed tube helium compressor offers temperature control in the range of 5 K to 300 K. Variable and static electric field can be applied for stroboscopic study of ferroelectric materials. The wide neutron wavelength band is well suited for efficient 3D Q space mapping of Bragg and diffuse scattering originating from magnetic and nuclear interactions simultaneously. TOPAZ samples can be oriented with high precision for volumetric sampling of Braggpeaks in specific directions. Currently, TOPAZ has 25 of 48 detector ports populated with Anger camera modules covering a scattering angle between 20° and 160° in 2θ, matching 3.2 sr in solid angle coverage. A full dataset for structure analysis can be collected with 4 to 25 settings with an exposure time of about 0.5–5 hours each, depending on the crystal symmetry, sample scattering strength, and crystal size.



APPLICATIONS

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

- Functional inorganic materials for studying the interplay of nuclear and magnetic structures such as doping-driven structural distortion in iridates; Fe and Co site occupancies in a molecular precursor
- Hydrogen bonding, guest-host interaction, and guest mobility in hydride perovskites; high-pressure synthesized mantle mineral and self-assembling tertiaryamines
- Catalytic and dihydrogen activation or exchange materials for the study of metal-hydrogen bonding in electrocatalyst and nano-sized copper clusters
- Accurate atomic position and displacement parameters for charge density study of organic crystals containing a high percentage of hydrogen atoms

SPECIFICATIONS

Moderator	Decoupled poisoned supercritical hydrogen
Source-to-sample distance	18 m
Sample-to-detector distance	39–46 cm
Angular detector coverage	3.2 sr (25 detectors)
Detector size	15 × 15 cm^2 with 256 by 256 pixels
Detector angular range	20–160° 2θ; ± 32° out-of-plane
Wavelength bandwidth	3.1 Å
Frame 1	0.4–3.5 Å
d-Spacing Q-range	0.25–14 Å 0.45–25 $Å^{-1}$
Sample size	> 0.05 mm^3 in volume and > 0.1 mm on an edge
Average experiment time	4 days / 1 complete data set
Neutron beam sizes	2.0–5.0 mm diameter
Sample environment	Ambient goniometer: 90–450 K Cryogenic goniometer: 5–300 K

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For more information, contact

Xiaoping Wang, wangx@ornl.gov, 865.576.2148
Christina Hoffmann, choffmann@ornl.gov, 865.576.5127

neutrons.ornl.gov/topaz

Oak Ridge National Laboratory
Managed by UT-Battelle LLC
for the US Department of Energy