Neutron Diffractometers at HFIR and SNS (ORNL)

Stuart Calder

Oak Ridge National Laboratory,

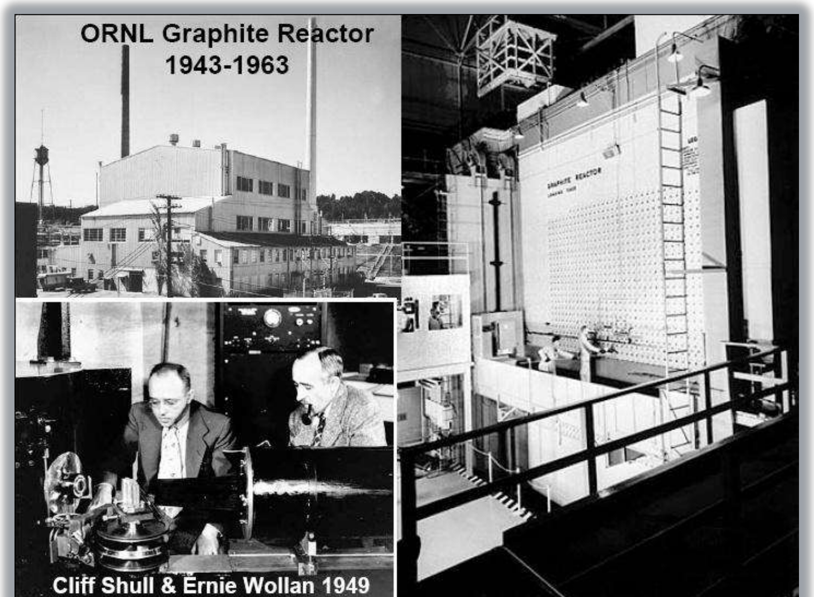
High Flux Isotope Reactor (HFIR)

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

First magnetic neutron diffraction performed at Oak Ridge National Laboratory (ORNL)

- Clifford G. Shull received 1994 Nobel prize in Physics.



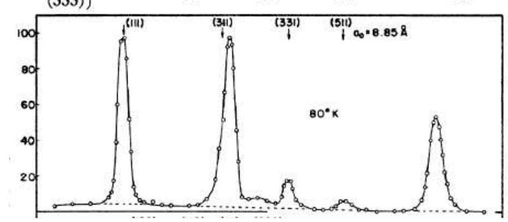
PHYSICAL REVIEW VOLUME 83, NUMBER 2 JULY 15, 1951

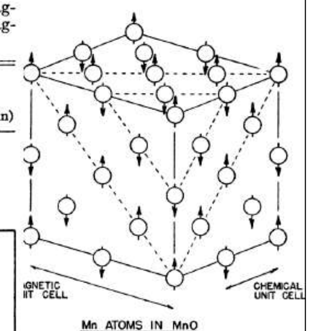
Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

C. G. Shull, W. A. Strauser, and E. O. Wollan
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received March 2, 1951)

Table II. Comparison between observed MnO antiferromagnetic intensities and those calculated for various models of magnetic orientation with respect to crystallographic axes.

	(100) (a)	(111) (b)	⊥[111] (c)	Observed (neutrons/min)
(111)	1038	0	1560	1072
(311)	460	675	...	308
(331)	129	109	...	132
(511) (333)	54	24	...	70





- First direct evidence of antiferromagnetism in MnO.
- Neel model of ferrimagnetism confirmed in Fe_3O_4.
- First magnetic form-factor data obtained in Mn compounds.
- Production of polarized neutrons by Bragg reflection from ferromagnets demonstrated.

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR

Oak Ridge National Laboratory (ORNL)

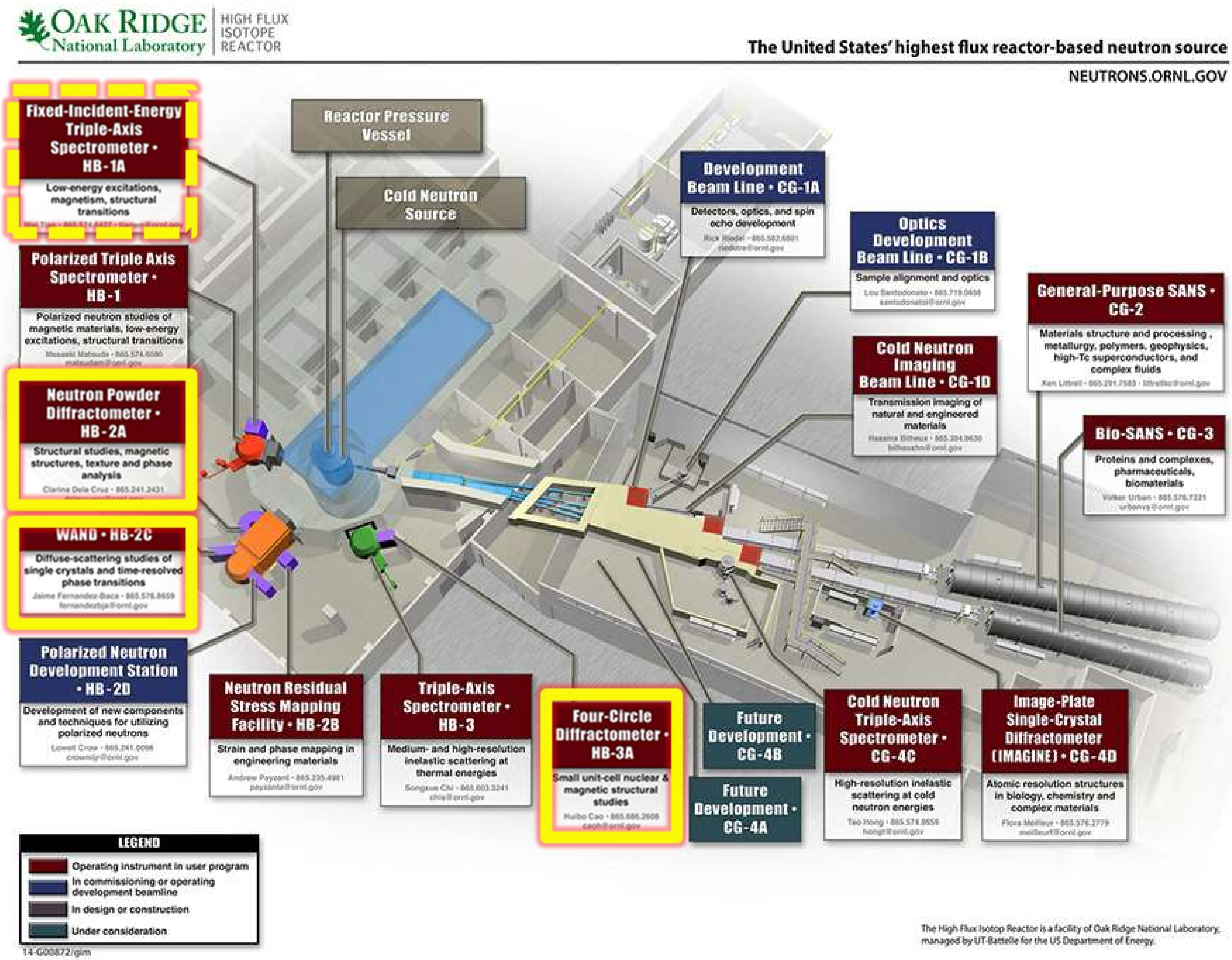
- **Neutrons:** High Flux Isotope Reactor (HFIR)
  Spallation Neutron Source (SNS)

- Neutrons produced from a reactor core.
- Highest flux reactor based source in the U.S. (80 MW)

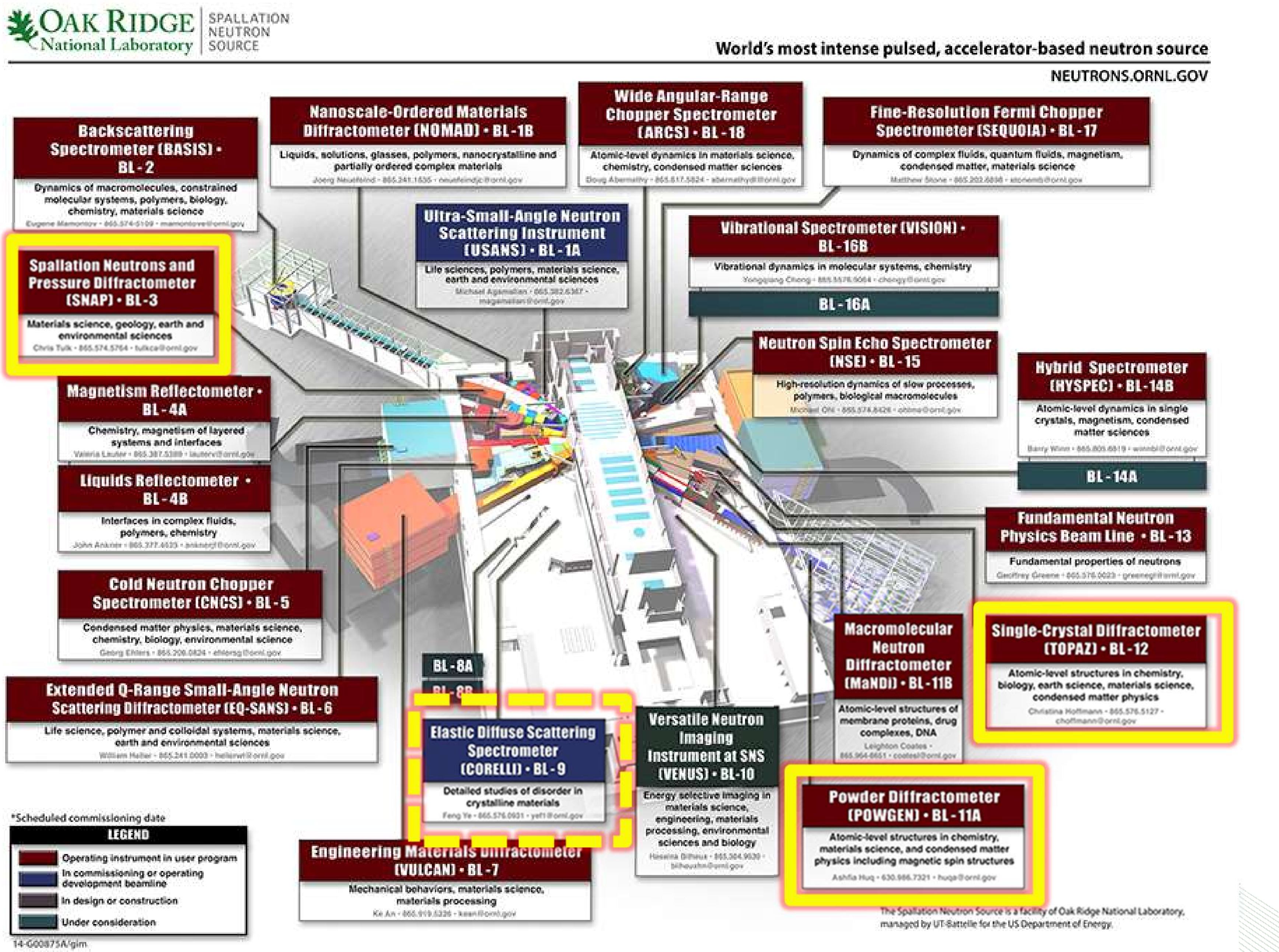
- Neutrons produced from an accelerator.
- Most intense pulsed neutron beam. (60Hz, 1.4 MW)

- Several complimentary diffraction beamlines at ORNL.
- Science of the material will dictate choice of instrument(s).
- Second target station will add further capabilities.

HFIR


OAK RIDGE National Laboratory
HIGH FLUX ISOTOPE REACTOR
The United States' highest flux reactor-based neutron source
NEUTRONS.ORNL.GOV
Fixed-Incident-Energy Triple-Axis Spectrometer • HB-1A
Low-energy excitations, magnetism, structural transitions
Polarized Triple Axis Spectrometer • HB-1
Polarized neutron studies of magnetic materials, low-energy excitations, structural transitions
Neutron Powder Diffractometer • HB-2A
Structural studies, magnetic structures, texture and phase analysis
WAND • HB-2C
Diffuse-scattering studies of single crystals and time-resolved phase transitions
Polarized Neutron Development Station • HB-2D
Development of new components and techniques for utilizing polarized neutrons
Neutron Residual Stress Mapping Facility • HB-2B
Strain and phase mapping in engineering materials
Triple-Axis Spectrometer • HB-3
Medium- and high-resolution inelastic scattering at thermal energies
Four-Circle Diffractometer • HB-3A
Small unit-cell nuclear & magnetic structural studies
Reactor Pressure Vessel
Cold Neutron Source
Development Beam Line • CG-1A
Detectors, optics, and spin echo development
Optics Development Beam Line • CG-1B
Sample alignment and optics
Cold Neutron Imaging Beam Line • CG-1D
Transmission imaging of natural and engineered materials
General-Purpose SANS • CG-2
Materials structure and processing, metallurgy, polymers, geophysics, high-Tc superconductors, and complex fluids
Bio-SANS • CG-3
Proteins and complexes, pharmaceuticals, biomaterials
Future Development • CG-4B
Future Development • CG-4A
Cold Neutron Triple-Axis Spectrometer • CG-4C
High-resolution inelastic scattering at cold neutron energies
Image-Plate Single-Crystal Diffractometer (IMAGINE) • CG-4D
Atomic resolution structures in biology, chemistry and complex materials
LEGEND
Operating instrument in user program
In commissioning or operating development beamline
In design or construction
Under consideration
14-G00872/gim
The High Flux Isotop Reactor is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

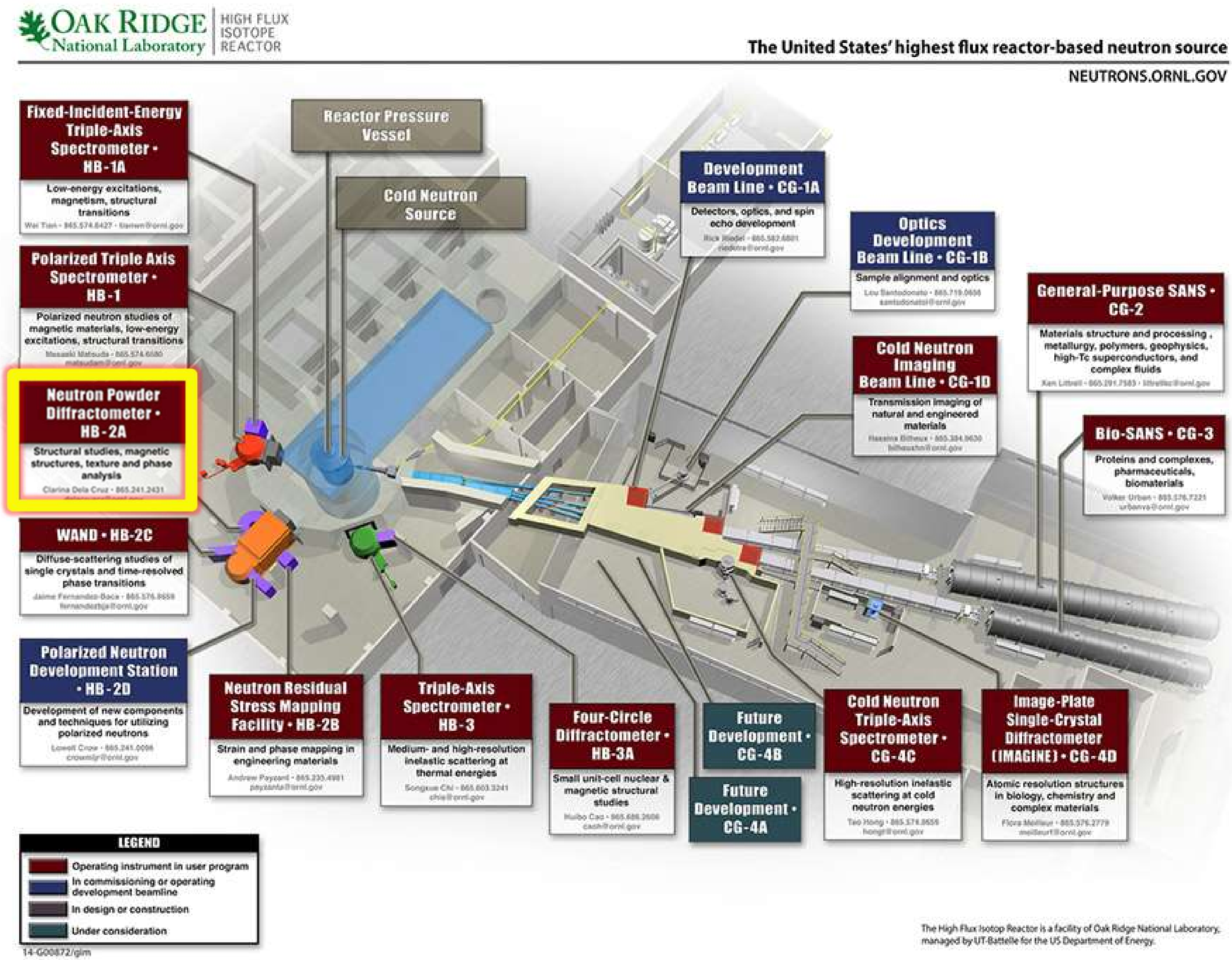
SNS



OAK RIDGE National Laboratory
SPALLATION NEUTRON SOURCE
World's most intense pulsed, accelerator-based neutron source
NEUTRONS.ORNL.GOV
Backscattering Spectrometer (BASIS) • BL-2
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Nanoscale-Ordered Materials Diffractometer (NOMAD) • BL-1B
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Wide Angular-Range Chopper Spectrometer (ARCS) • BL-18
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) • BL-17
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Ultra-Small-Angle Neutron Scattering Instrument (USANS) • BL-1A
Life sciences, polymers, materials science, earth and environmental sciences
Vibrational Spectrometer (VISION) • BL-16B
Vibrational dynamics in molecular systems, chemistry
BL-16A
Spallation Neutrons and Pressure Diffractometer (SNAP) • BL-3
Materials science, geology, earth and environmental sciences
Neutron Spin Echo Spectrometer (NSE) • BL-15
High-resolution dynamics of slow processes, polymers, biological macromolecules
Hybrid Spectrometer (HYSPEC) • BL-14B
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
BL-14A
Magnetism Reflectometer • BL-4A
Chemistry, magnetism of layered systems and interfaces
Liquids Reflectometer • BL-4B
Interfaces in complex fluids, polymers, chemistry
Fundamental Neutron Physics Beam Line • BL-13
Fundamental properties of neutrons
Cold Neutron Chopper Spectrometer (CNCS) • BL-5
Condensed matter physics, materials science, chemistry, biology, environmental science
Macromolecular Neutron Diffractometer (MaNDi) • BL-11B
Atomic-level structures of membrane proteins, drug complexes, DNA
Single-Crystal Diffractometer (TOPAZ) • BL-12
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
BL-8A
BL-8B
Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) • BL-6
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
Elastic Diffuse Scattering Spectrometer (CORELLI) • BL-9
Detailed studies of disorder in crystalline materials
Versatile Neutron Imaging Instrument at SNS (VENUS) • BL-10
Energy selective imaging in materials science, engineering, materials processing, environmental sciences and biology
Powder Diffractometer (POWGEN) • BL-11A
Atomic-level structures in chemistry, materials science, and condensed matter physics including magnetic spin structures
Engineering Materials Diffractometer (VULCAN) • BL-7
Mechanical behaviors, materials science, materials processing
*Scheduled commissioning date
LEGEND
Operating instrument in user program
In commissioning or operating development beamline
In design or construction
Under consideration
14-G00875A/gim
The Spallation Neutron Source is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

Powder diffraction

HFIR



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14-G00872/gim
The High Flux Isotop Reactor is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

HB-2A Powder diffractometer (HFIR)

- Constant wavelength diffractometer: λ=2.41 Å or 1.54 Å
- 2theta range 3 deg to 155 deg.
- Available for users since 2009.
- Focus is magnetic diffraction, balance between intensity and resolution.
- Clean background ideal for magnetism and complex sample environments.

Our user base in 2009-2013

Sample environments (HB-2A)

Low Temperature

- Conventional closed cycle refrigerators (CCR) 4 K – 700 K.
- ^{4}He crystats (1.5 K – 300 K)
- ^{3}He-^{4}He dilution (27 millikelvin)

High Magnetic fields

- 5 T standard (16 T and pulsed available on other beamlines)
- Can combine 27 mK with 5 T.

High Pressures

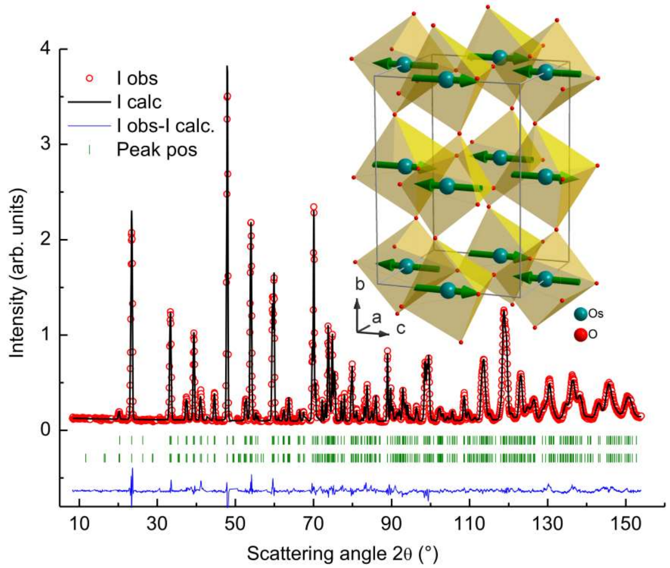
- HB-2A offers Clamp cells (2 GPa) and Fluid/gas cells (10 kbar)
- Dedicated beamline (SNAP) with diamond anvil cells (to 100 Gpa)

Polarized neutrons on HB-2A

- Incident polarized beam available for ferromagnetic and ferrimagnetic studies.

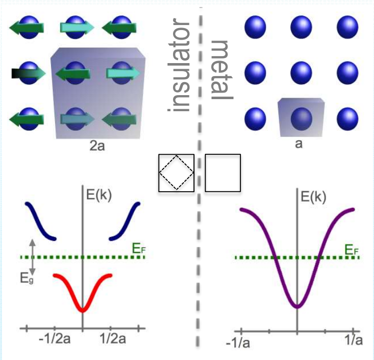
Neutrons confirm long predicted metal-insulator transition theory

Slater MIT mechanism demonstrated in $NaOsO_3$ on HB-2A diffractometer



Neutron diffraction data modeled with the G-type antiferromagnetic order that is responsible for driving the metal insulator transition in $NaOsO_3$

Schematic of the Slater mechanism.

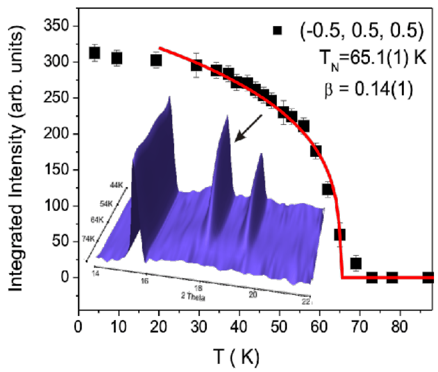


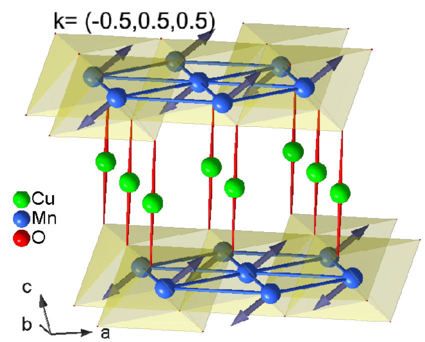
- The metal-insulator transition (MIT), of both fundamental and technological interest, is one of the most dramatic manifestations of electron correlations in materials.
- Several mechanisms that produce MITs have been considered over the years, including Mott (electron localization via Coulomb repulsion), Anderson (localization via disorder), and Peierls (localization via distortion of a one-dimensional lattice).
- A mechanism proposed by Slater in 1951, in which long-range magnetic order drives the MIT, has remained elusive.
- Neutron scattering at the Neutron Powder Diffractometer and Polarized Triple-Axis Spectrometer at the High Flux Isotope Reactor, along with x-ray scattering at the Advanced Photon Source, were used to probe the 5d transition metal oxide $NaOsO_3$.
- The experiments uncovered the Slater mechanism for magnetic ordering in $NaOsO_3$ and are the first definitive demonstration of this long-predicted MIT.

S. Calder et al., PRL 108 257209 (2012)

$Cu(Mn_{1-x}Cu_x)O_2$: Tuning of Magnetism by chemical substitution

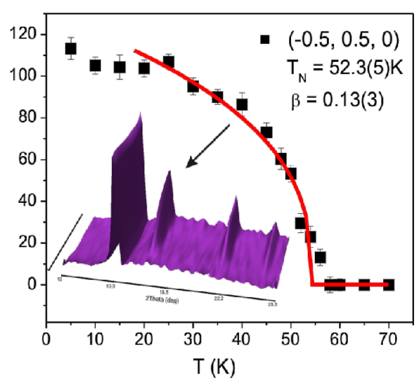
$CuMnO_2$

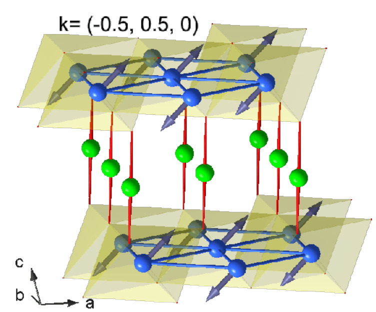


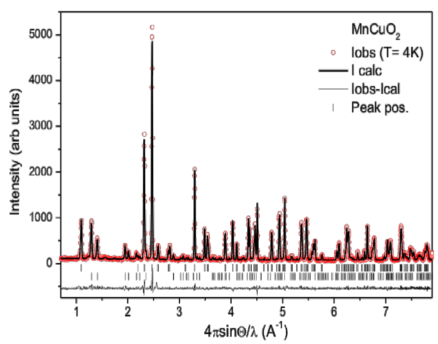


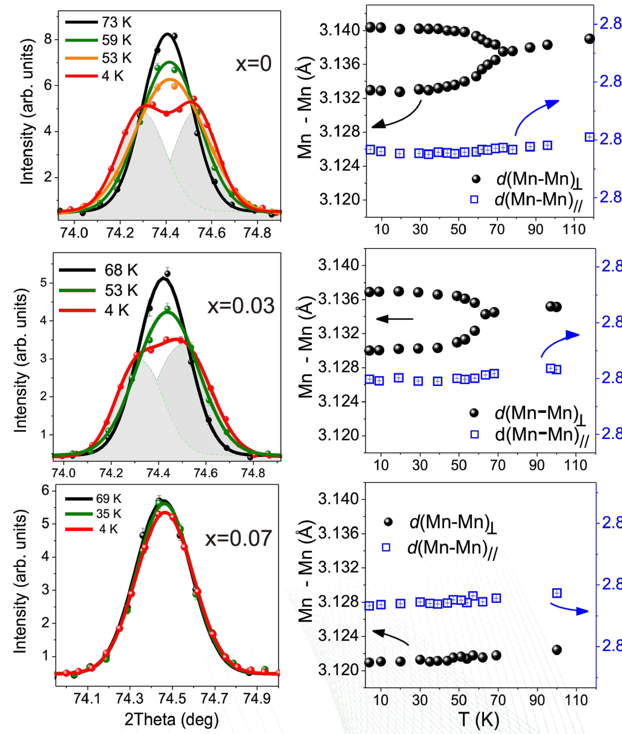
$Cu(Mn_{1-x}Cu_x)O_2$: Magneto-elastic transition

$Cu(Mn_{0.93}Cu_{0.07})O_2$





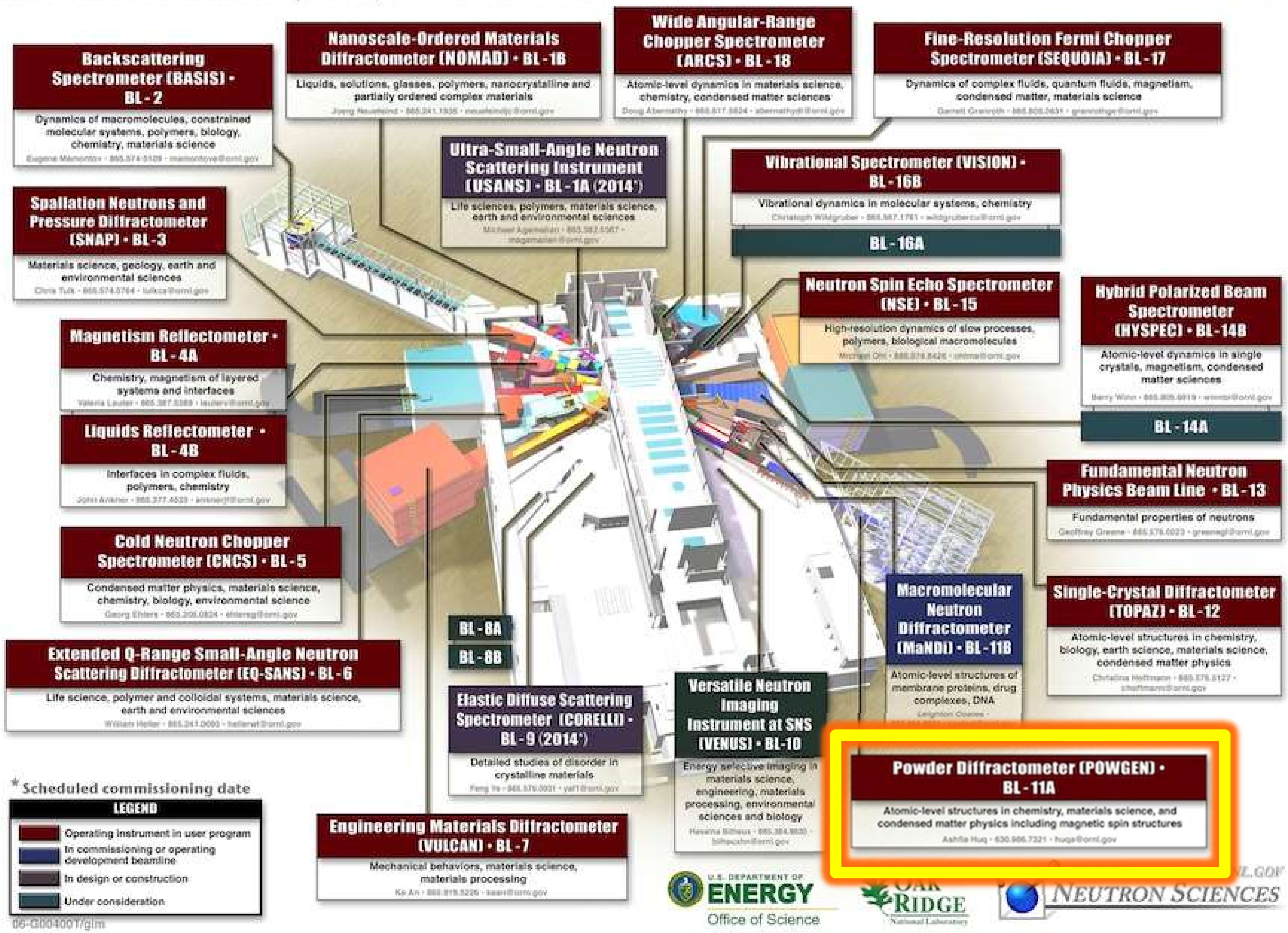




• V. O. Garlea *et al.*, PRB 83, 172407 (2011)

Spallation Neutron Source at Oak Ridge National Laboratory

The world's most intense pulsed, accelerator-based neutron source



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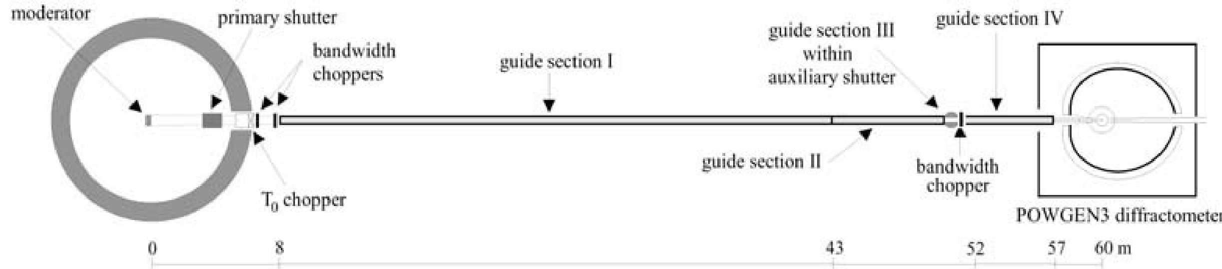
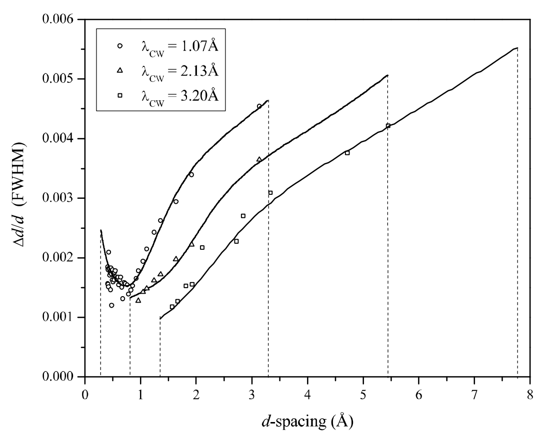
NEUTRON SCIENCES

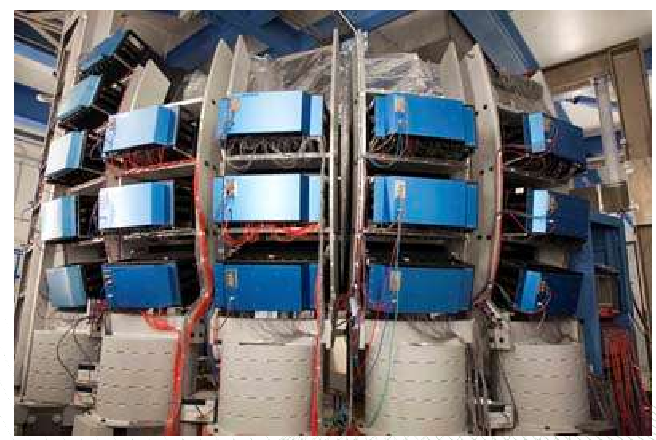
POWGEN (SNS)



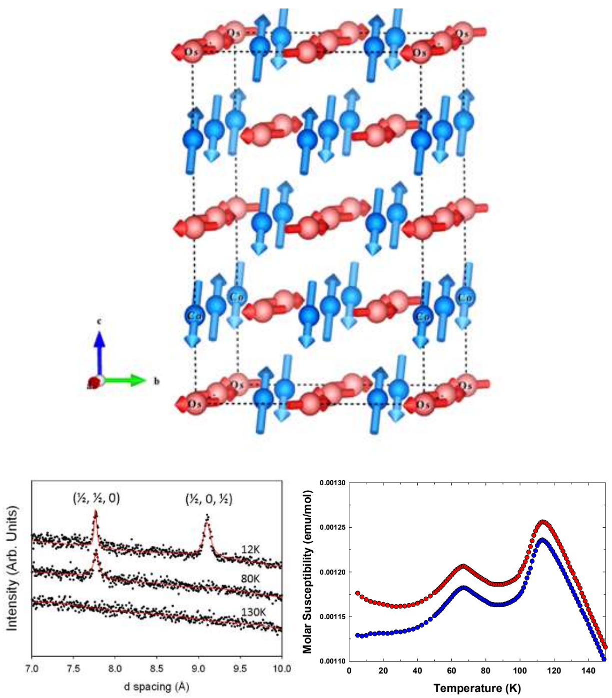
- General purpose diffractometer that encompasses magnetic scattering.
- Optimized for crystal structure determination.
- Alternative design to previous spallation diffractometers
  → data reduced to single pattern.
- Different wavelengths (Frames) available. Magnetic Frame: Q= 0.4 Å^{-1} to 3 Å^{-1}
  Generally a wide detector angular coverage 20<2Θ<159
- Currently optimized for high Q, but more low angular detector coverage planned.

Instrument resolution





Neutrons Discover Unusually Strong Long Range Superexchange Interactions in Mixed Transition Metal Oxides



Magnetic Structure of Sr_2CoOsO_6 at low temperatures (top), key magnetic reflcection corresponding to independent ordering of Os and Co sublattices (bottom left), and SQUID data indicating two antiferromagnetic transitions (bottom right)

Work was performed at the ORNL Spallation Neutron Source's POWGEN instrument.

Scientific Achievement

Neutron powder diffraction on double perovskite Sr_2CoOsO_6 reveals a magnetic structure in which the two magnetic sublattices order independently at different temperatures via four bond superexchange pathways.

Significance and Impact

These results provide important information for designing magnetic materials with magnetic transition metals from differing rows of the periodic table, a situation where the long standing Goodenough-Kanamori rules fail to apply.

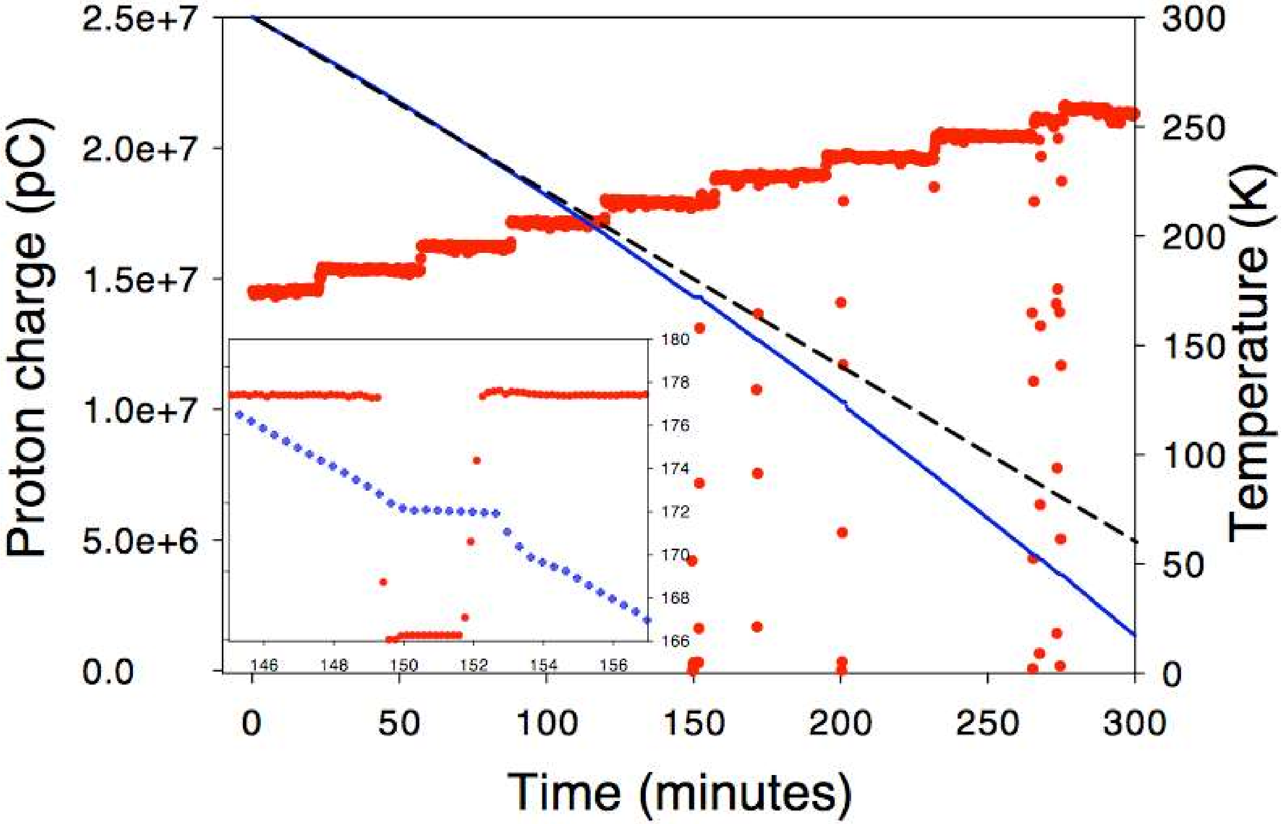
Research Details

- Os spins order at 108K via a ferromagnetic Os-O-Co-O-Os exchange pathway while Co spins order at 70K via an antiferromagnetic Co-O-Os-O-Co exchange pathway
- Complimentary DFT calculations find that typically dominant nearest neighbor Co-O-Os exchange is an order of magnitude weaker, resulting in decoupled sublattices

R. Morrow, R Mishra, O.D. Restrepo, M.R. Ball, W. Windl, S. Wurmehl, U. Stockert, B. Büchner, P.M. Woodward. Journal of the American Chemical Society **2013** (accepted)

Magnetite (Fe3O4)

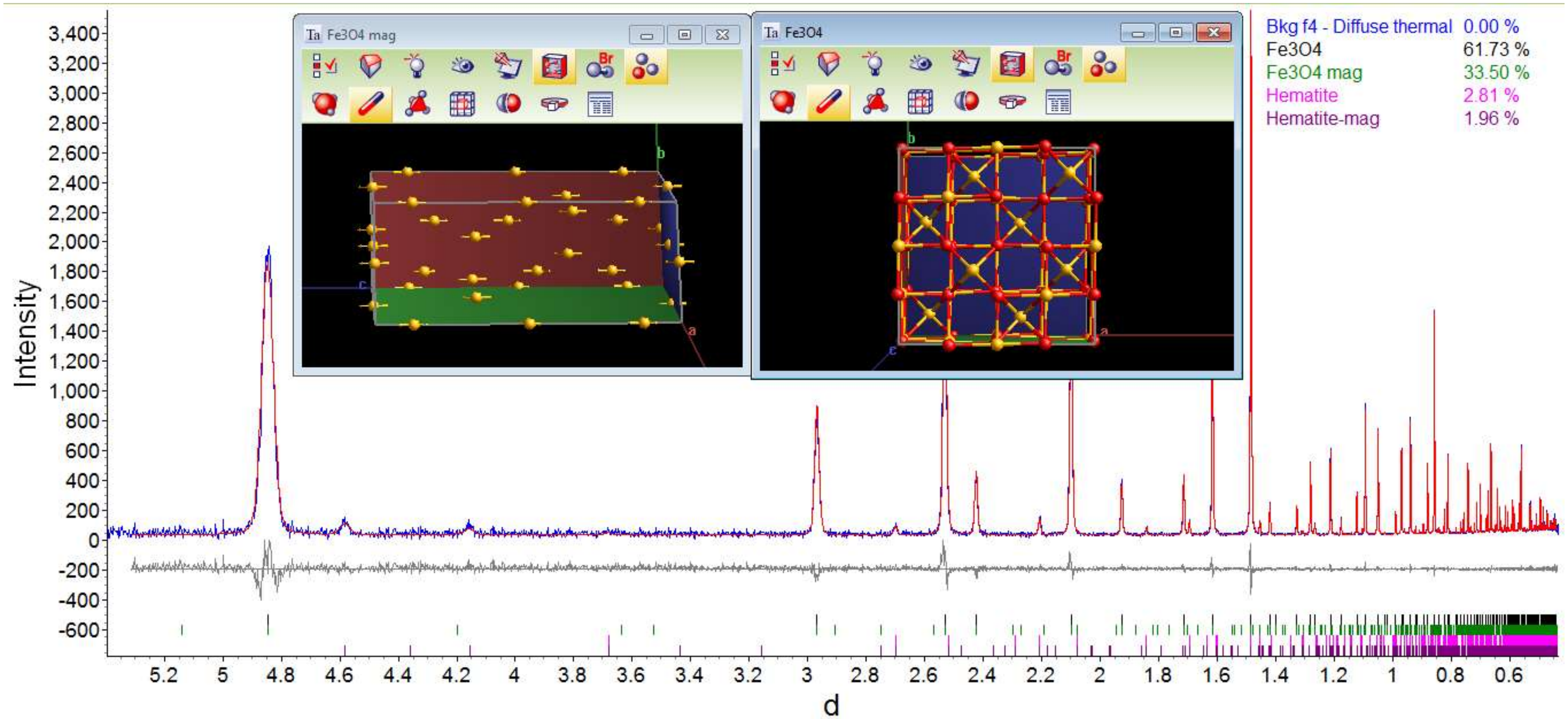
- Sample cooled down to 10 K at a nominal 1 K/minute
- Temperature controlled for a near constant DT/D(pcharge) = constant counting statistics
- Ramping accelerates with increasing beam power & halts when it trips



Plot of proton charge and controller set-point during data collection on Fe3O4.

Using sliced data....

- Temperature sliced data perfectly usable for refinement….
- Extension to parametric studies a logical step



Magnetic structure refinement of Fe_3O_4 at 295 K with a 5 K slice (nominally 5 minutes) of the ramping data

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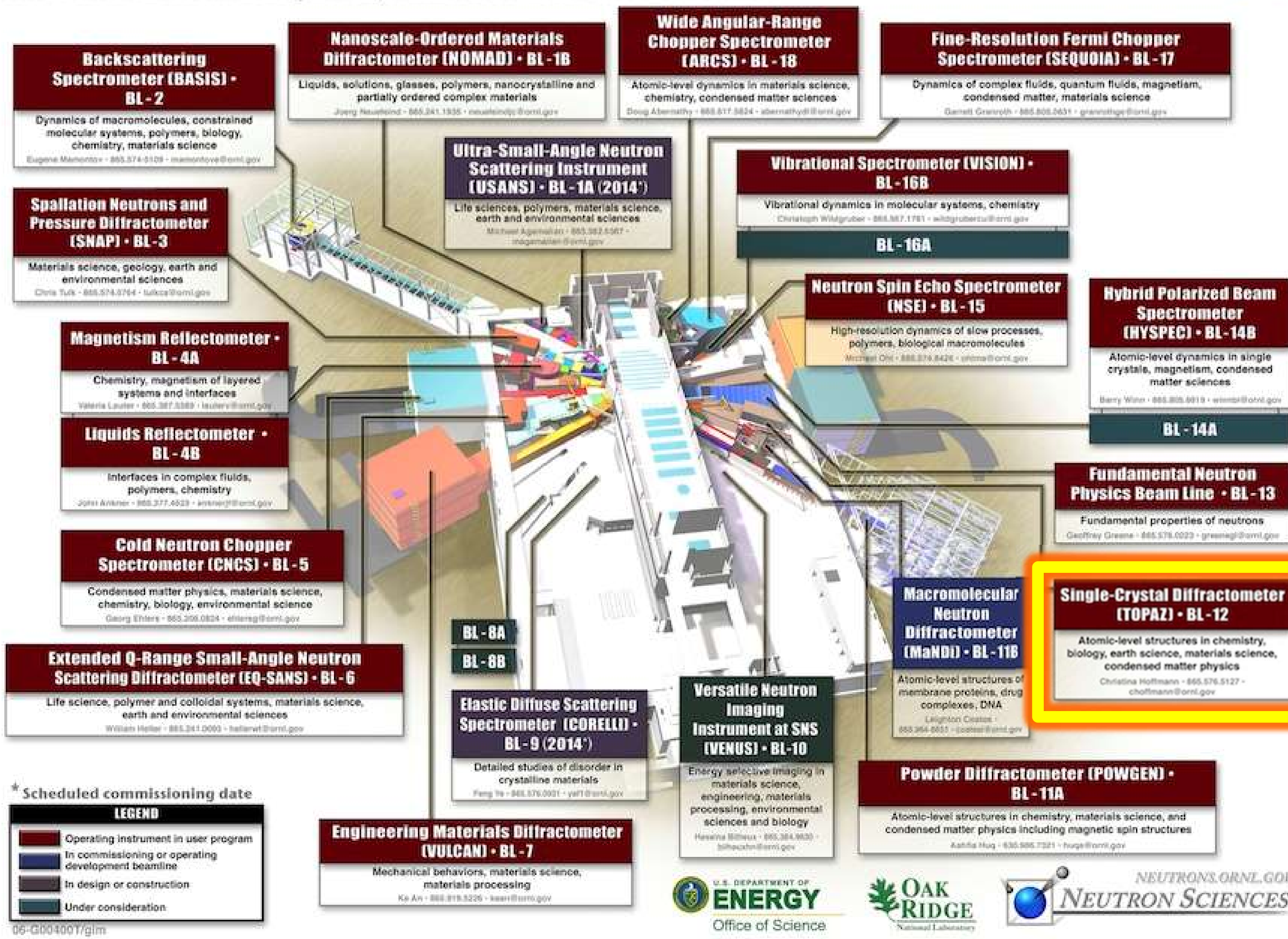
Single crystal diffraction

Spallation Neutron Source at Oak Ridge National Laboratory

The world's most intense pulsed, accelerator-based neutron source



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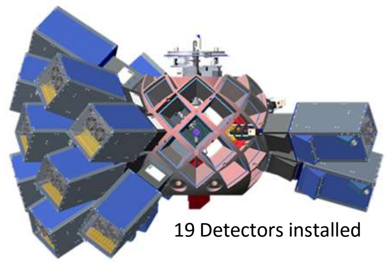
TOPAZ (SNS BL-12): Single crystals

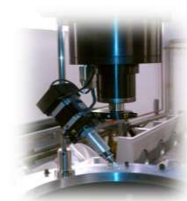
Instrument Parameter

Moderator	decoupled poisoned super critical H_2
Source to sample	18 m
Sample to detector	0.395-0.460 m
Detector angular coverage	13.5°< 2Θ <160°
Detector solid angle coverage	2.4 ster.
Bandwidth	~3.6 Å
Frames 1 & 2 (λ range at 60Hz)	0.25 - 3.85 Å; 3.9 - 7.1 Å
Sample size: Diameter, Volume	0.05 - 2.5 mm, >0.10 mm³
Unit cell length, Resolution	<70 Å, d_{min}>= 0.4 Å

Sample Environment

- ❑ Crystal Logic Goniostat : Fixed chi at 135° with 360° rotations in omega and phi
- ❑ CryoStream 700Plus: 90 K-500 K
- ❑ Upgrade – Cryogenic Goniometer: 5 K to 295 K

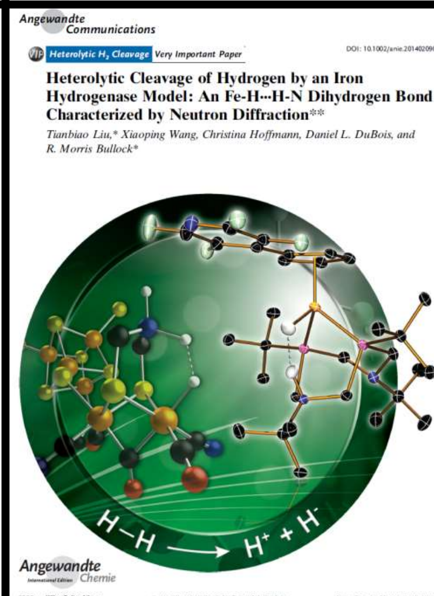

19 Detectors installed


Crystal Logic Goniostat raised for sample mount

Primary Usage

TOPAZ is a high resolution time-of-flight Laue diffractometer. It is capable of measuring a 3*D* volume of reciprocal space during each pulse from a *small* stationary single crystal using an array of state-of-the-art neutron area detectors with sub-microsecond readout time for individual neutron events.

- ❑ **Chemical crystallography complementary to X-rays**
- ❑ **Magnetic structure**
- ❑ **Diffuse scattering**
- ❑ **Neutron event-based parametric study of nuclear and magnetic structural phase transitions**



Science Highlight

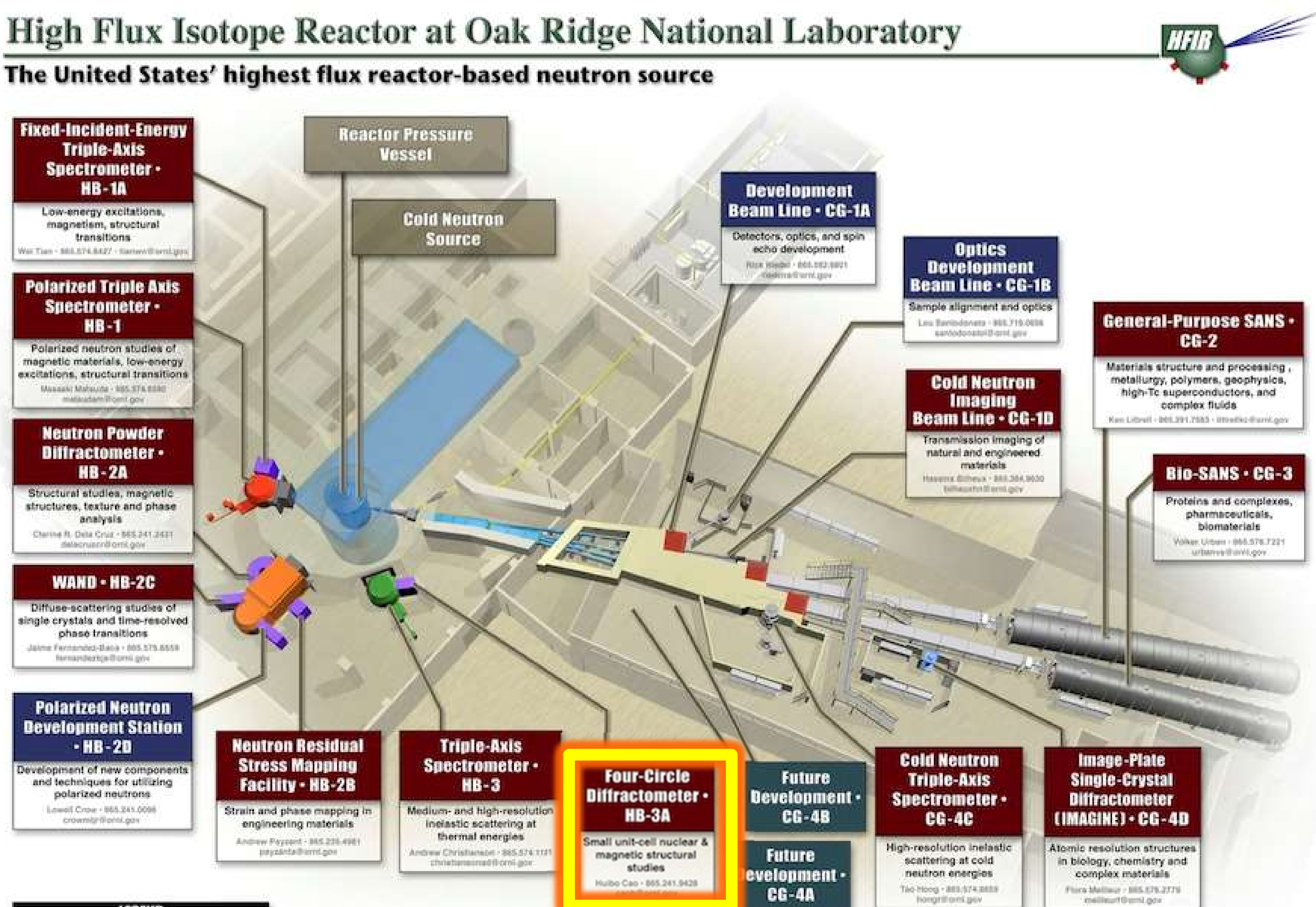
The structure of an Fe-based electrocatalyst mimicking the [FeFe]-hydrogenase was determined from neutron diffraction. Single-crystal neutron diffraction reveals the first time a unusually strong acidic N-$H^{\delta+}$ and hydridic Fe-H^{δ} hydrogen bonding interaction resulted from the heterolytic cleavage of H_2, and provides insight into making more efficient electrocatalyst for the oxidation of H_2 in fuel cells.

T. Liu, X. Wang, C. Hoffmann, D.L. DuBois and R.M. Bullock, *Angew. Chem. Int. Ed.* 53 (2014) 5300-5304.

JANA2006 can now read TOPAZ data and apply neutron wavelength-dependent extinction correction for TOF Laue data with direction cosines.

High Flux Isotope Reactor at Oak Ridge National Laboratory

The United States' highest flux reactor-based neutron source



LEGEND

- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

07-G00244N/gim

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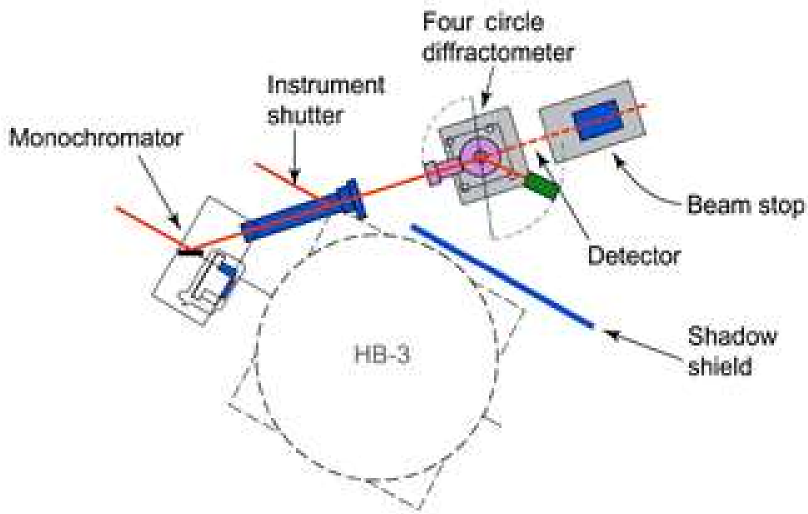
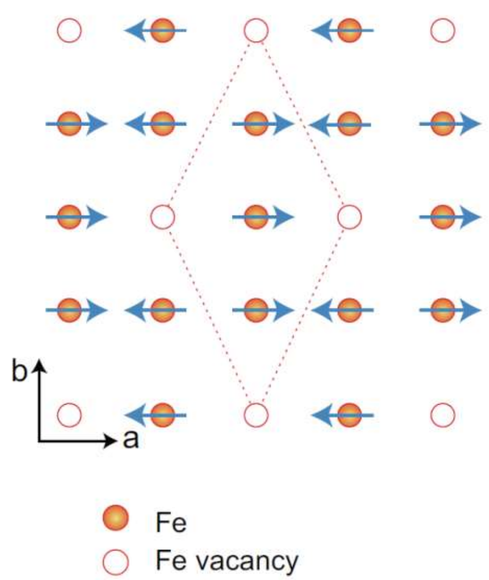
Four-circle diffractometer (HB-3A)

- Beam size of $6x8mm^2$ → minimum crystal of $1mm^3$
- 2D detector and single-point ^3He detector
- Choice of incident wavelengths from vertical focusing Si monochromator: 1.0 Å, 1.54 Å and 2.54 Å
- Full χ circle goniometer.



A New Direction for Iron-Based Superconductors



Stripe-type magnetic order and rhombus iron vacancy order of semiconducting $K_{0:85}Fe_{1:54}Se_2$. The red dashed line marks the 2 × 4 rhombus iron vacancy order.

J. Zhao, H. Cao, E. Bourret-Courchesne, D.-H. Lee, R. J. Birgeneau, Phys. Rev. Lett., **2012**, *109*, 267003.

Work was performed at the HFIR Four-Circle Diffractometer.

Scientific Achievement

Single-crystal neutron diffraction is a powerful means of determining magnetic structures. In this study, the technique was used to show that the parent phase of superconductors in the $K_xFe_{2-y}Se_2$ family has a novel magnetically ordered semiconducting ground state.

Significance and Impact

This research opens new avenues for comprehending the magnetism of iron-based superconductors and sets a new direction in the search for magnetic high-temperature superconductors.

Research Details

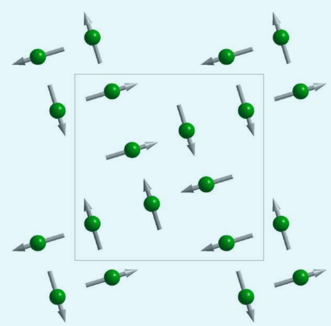
– Superconductivity was introduced by electron doping, which suppresses the stripe AF order, leading to a magnetic phase diagram similar to those of cuprates and iron pnictides.

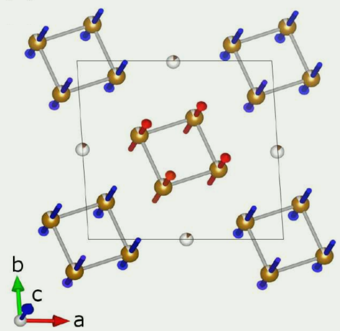
– Neutron diffraction was used to study the structure, magnetic order, and stoichiometry of single crystals of $K_xFe_{2-y}Se_2$ compounds.

Spin Reorientation in $TlFe_{1.6}Se_2$ with Complete Vacancy Ordering

Ordered vacancies tune the magnetic order.

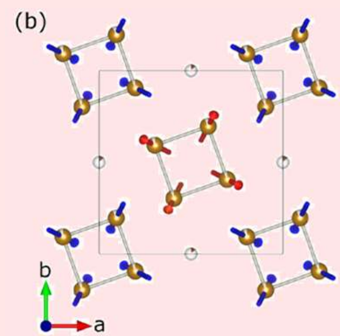
NC: non-collinear AFM structure with spins lying in *ab*-plane

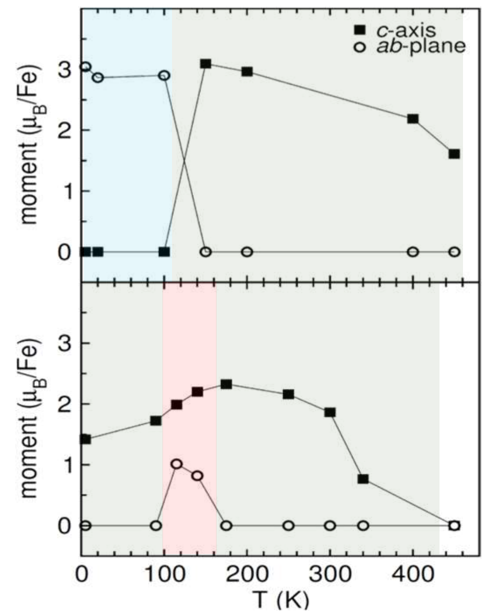




BC: block-checkerboard structure with spins aligned with *c*-axis.

Canted: spins in BC develop an *ab*-plane component of the moment



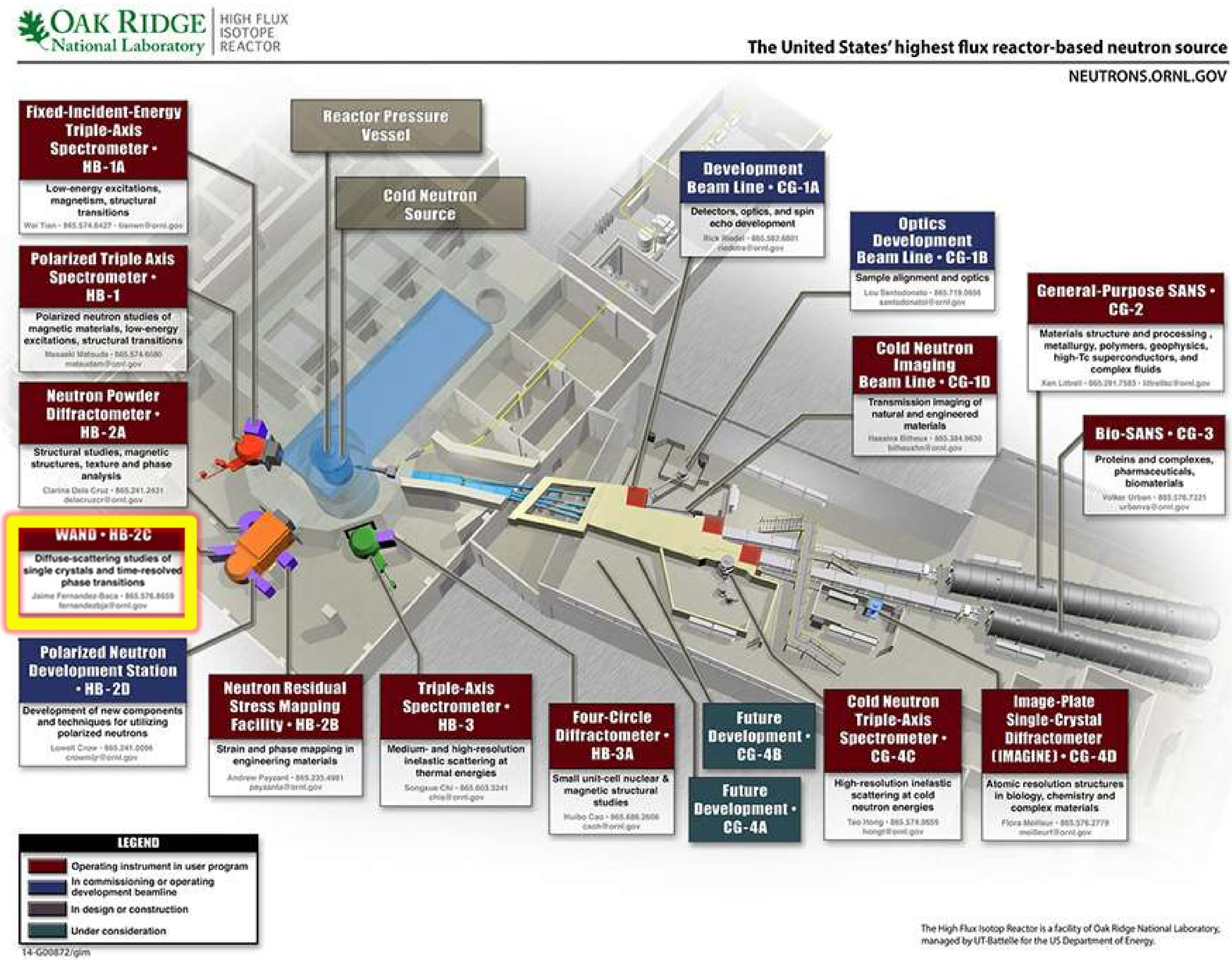


- Detailed characterization of single crystal $TlFe_{1.6}Se_2$ with complete chemical and vacancy order reveals a previously unobserved spin reorientation with spins lying in the ab plane for T < 100 K.
- A strong interaction between the ordered and disordered regions must prevent this ground state from occurring in the partially disordered crystals at low temperatures.
- Single-crystal neutron diffraction was used at the HB-3A four-circle diffractometer, High Flux Isotope Reactor, ORNL, to determine these magnetic structures as a function of temperature.

May et al., *Physical Review Letters*, 109, 077003 (2012)

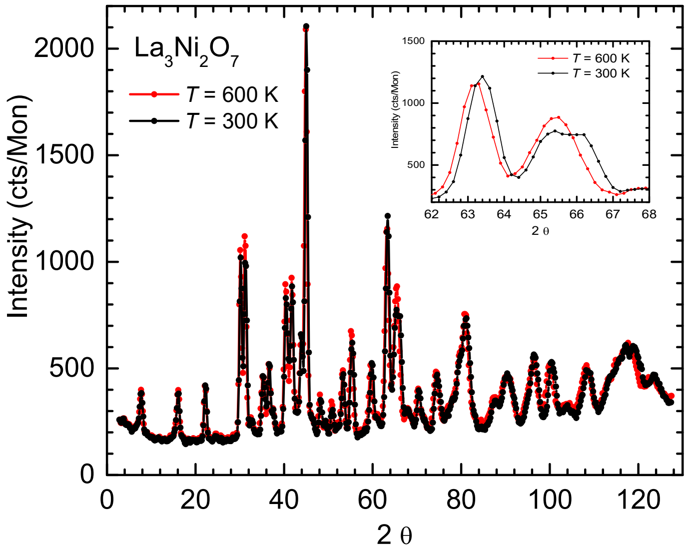
Powder and/or single crystal diffraction

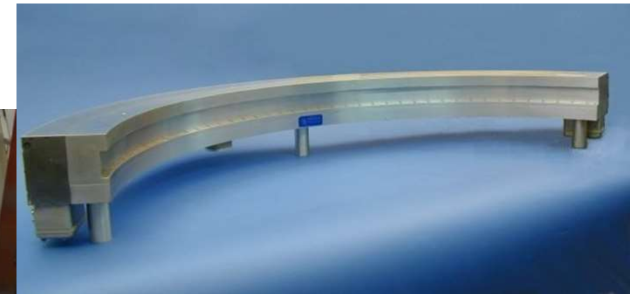
HFIR



OAK RIDGE National Laboratory
HIGH FLUX ISOTOPE REACTOR
The United States' highest flux reactor-based neutron source
NEUTRONS.ORNL.GOV
Fixed-Incident-Energy Triple-Axis Spectrometer • HB-1A
Low-energy excitations, magnetism, structural transitions
Reactor Pressure Vessel
Cold Neutron Source
Development Beam Line • CG-1A
Detectors, optics, and spin echo development
Optics Development Beam Line • CG-1B
Sample alignment and optics
General-Purpose SANS • CG-2
Materials structure and processing, metallurgy, polymers, geophysics, high-Tc superconductors, and complex fluids
Polarized Triple Axis Spectrometer • HB-1
Polarized neutron studies of magnetic materials, low-energy excitations, structural transitions
Cold Neutron Imaging Beam Line • CG-1D
Transmission imaging of natural and engineered materials
Neutron Powder Diffractometer • HB-2A
Structural studies, magnetic structures, texture and phase analysis
Bio-SANS • CG-3
Proteins and complexes, pharmaceuticals, biomaterials
WAND • HB-2C
Diffuse-scattering studies of single crystals and time-resolved phase transitions
Polarized Neutron Development Station • HB-2D
Development of new components and techniques for utilizing polarized neutrons
Neutron Residual Stress Mapping Facility • HB-2B
Strain and phase mapping in engineering materials
Triple-Axis Spectrometer • HB-3
Medium- and high-resolution inelastic scattering at thermal energies
Four-Circle Diffractometer • HB-3A
Small unit-cell nuclear & magnetic structural studies
Future Development • CG-4B
Future Development • CG-4A
Cold Neutron Triple-Axis Spectrometer • CG-4C
High-resolution inelastic scattering at cold neutron energies
Image-Plate Single-Crystal Diffractometer (IMAGINE) • CG-4D
Atomic resolution structures in biology, chemistry and complex materials
LEGEND
Operating instrument in user program
In commissioning or operating development beamline
In design or construction
Under consideration
14-G00872/gim
The High Flux Isotop Reactor is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

WAND





- **Vertical focusing hot-pressed Ge monochromator – λ = 1.48 Å (113) or λ = 0.94 Å (115) without significant higher order contamination.**

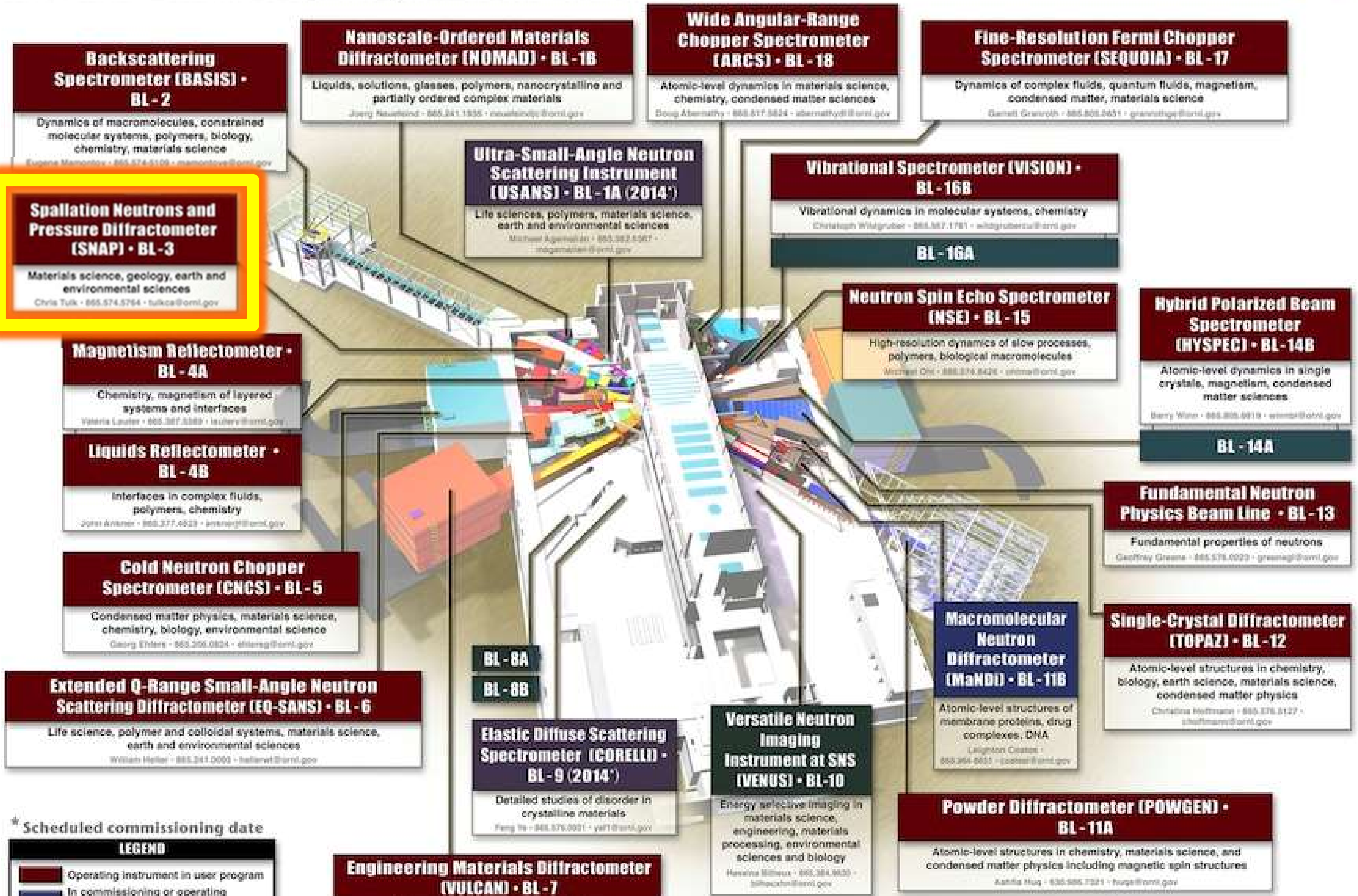
- **Medium-Resolution High intensity powder diffractometer – allows fast measurements for parametric studies.**

- **Continuous detector 1D position sensitive detectors. 624 anodes with 0.2 degree separation.**

- **Single crystal measurements: the good signal to noise ratio allows the detection of weak signals from superstructure, low dimensional magnetic order.**

Spallation Neutron Source at Oak Ridge National Laboratory

The world's most intense pulsed, accelerator-based neutron source



* Scheduled commissioning date

LEGEND
- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

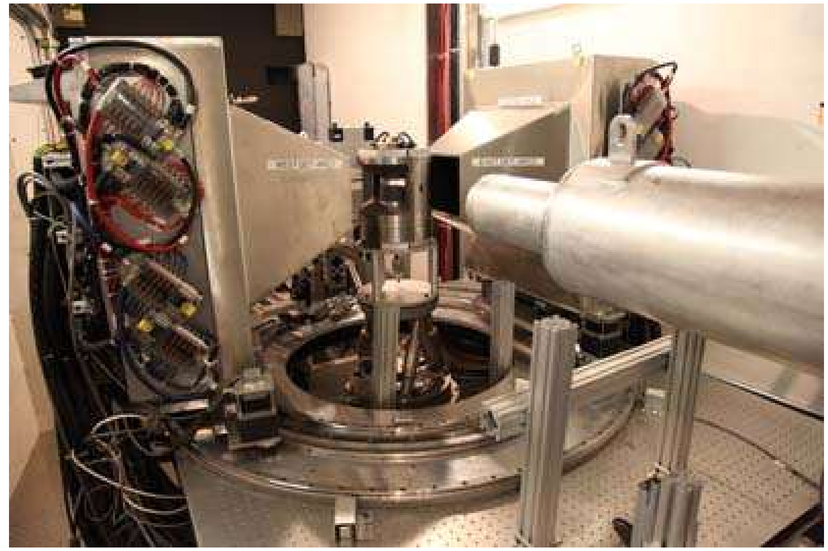
06-G00400T/glm

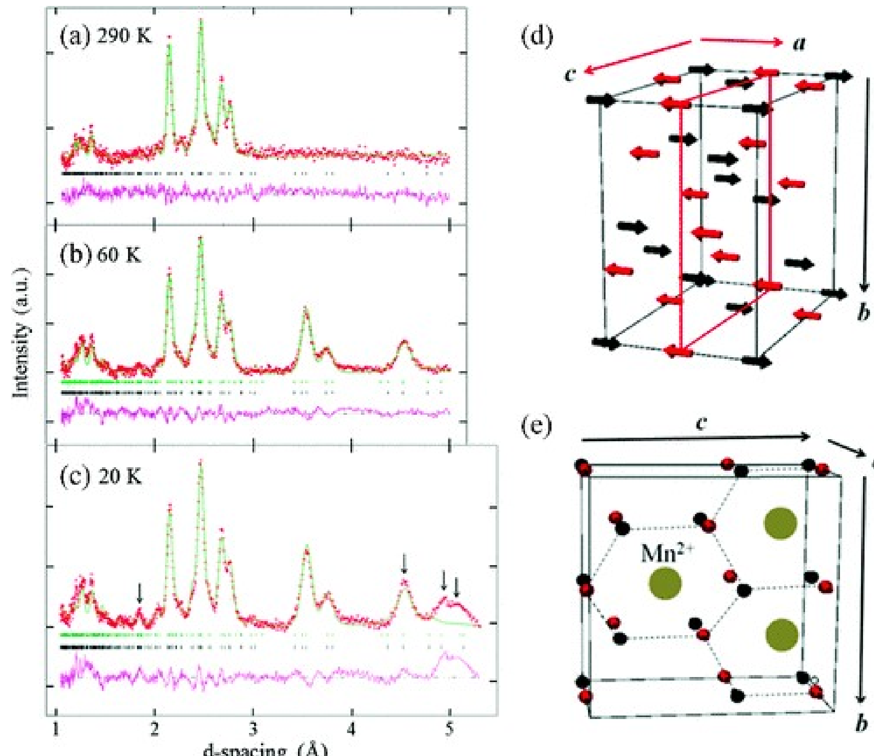
U.S. Department of Energy — Office of Science · Oak Ridge National Laboratory · NEUTRONS.ORNL.GOV Neutron Sciences

SNAP

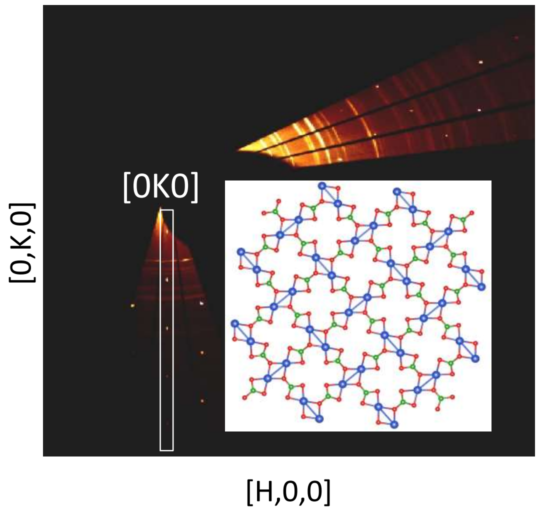
- Dedicated pressure beamline.
- Source to sample distance 15 m.
- Optimized for powders, crystals possible.
- Accessible Q as low as 0.78 Å^{-1}.
- Pressure 0-25 GPa at room temperature.
- 0-10 GPa between 85 and 300 K. Furnace also available.

S. Hirai, et al. “Giant atomic displacement at a magnetic phase transition in metastable Mn_3O_4” PRB 87 014417 (2013)

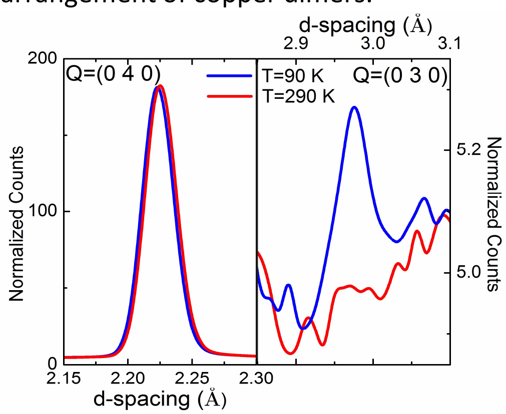




High-Pressure Single Crystal Diffraction Enables Unprecedented Measurements on Quantum Magnetic Materials on SNAP



Reciprocal space map of $SrCu_2(BO_3)_2$ collected at 5.5 GPa. (Inset) Depiction of the corresponding lattice plane, with a Shastry -Sutherland arrangement of copper dimers.



Temperature dependence of the [0K0] reflections. The [030] reflection is a factor of 400 weaker than the purely structural [040] reflection.

Scientific Achievement

In-Situ neutron scattering measurements of a single crystal under pressure reveal the magnetic structure resulting from the Antiferromagnetic Long Range Ordering in $SrCu_2(BO_3)_2$, a Shastry-Sutherland lattice model material. The Shastry-Sutherland model has played an influential role in developing the modern condensed matter physics field because it is sufficiently simple to be exactly soluble, but sufficiently rich to capture interesting physics.

Significance and Impact

The ability to measure data from single crystalline sample under high pressure (up to 100 KBar) enables researchers to reconcile the exploration of pressure as tuning parameter in quantum systems despite their characteristic weak magnetic signal.

Research Details

– A previously cut and aligned single crystal of $SrCu_2(BO_3)_2$ was loaded in a pressure cell able to cool the cell to 90K

– The precise alignment of the crystal and placement of the instrument detectors allowed the monitoring of the location where magnetic scattering is expected

– The highly localized scattering characteristic of single crystal diffraction allows the measurement of small reflections. Such experiments are inaccessible to standard powder diffraction.

Research performed at the SNAP Instrument at the Spallation Neutron Source, Oak Ridge National Laboratory

U.S. DEPARTMENT OF ENERGY | Office of Science

SNS SPALLATION NEUTRON SOURCE · McMaster University · THE UNIVERSITY OF CHICAGO · Argonne NATIONAL LABORATORY

Applying for beamtime at ORNL

- Two proposal calls per year (Spring/Fall)
- Next call and details: http://neutrons.ornl.gov/users/proposals.shtml
- SNS and HFIR in same proposal call.
- Contact instrument scientists to improve chances of beamtime!

POWGEN Mail In Program

- Proposals accepted continuously (not limited to general call).
- Temperatures between 10 K and 300 K.
- Maximum of 8 hours.
- http://neutrons.ornl.gov/powgen/mail-in-pgm.html