Neutron Experiments:

	Instrument	Beamline
N1-a	Triple-Axis Spectrometers	HFIR HB-1A
N1-b	Triple-Axis Spectrometers	HB-3
N2	Powder Diffractometer	HFIR HB-2A
N3	Four-Circle Diffractometer	HFIR HB-3A
N4	Neutron Imaging Station	HFIR CG-1D
N5-a	Small Angle Neutron Scattering	HFIR CG-2 General Purpose SANS
N5-b	Small Angle Neutron Scattering	HFIR CG-3 Bio-SANS
N5-c	Small Angle Neutron Scattering	SNS BL-6 EQ-SANS
N6	NOMAD Nanoscale-Ordered Materials Diffractometer	SNS BL-1B
N7	BASIS Backscattering Spectrometer	SNS BL-2
N8	SNAP Spallation Neutrons at Pressure	SNS BL-3
N9	Magnetism Reflectometer	SNS BL-4A
N10	Liquids Reflectometer	SNS BL-4B
N11	VULCAN Engineering Materials Diffractometer	SNS BL-7
N12	POWGEN Powder Diffractometer	SNS BL-11A
N13	ARCS Wide-Angular Range Chopper Spectrometer	SNS BL-18

Neutron Experiment Schedule:

Group	20-Aug	21-Aug	22-Aug	23-Aug
A	N6	N2	N13	N11
B	N2	N6	N11	N13
C	N5-a	N12	N8	N1-a
D	N4	N3	N9	N5-c
E	N3	N4	N5-c	N9
F	N12	N5-a	N1-a	N8
G	N9	N5-c	N4	N3
H	N5-c	N9	N3	N4
I	N8	N1-a	N5-a	N12
J	N1-a	N8	N12	N5-a
K	N13	N11	N6	N2
L	N5-b	N1-b	N10	N7
M	N11	N13	N2	N6
N	N10	N7	N5-b	N1-b
O	N7	N10	N1-b	N5-b
P	N1-b	N5-b	N7	N10

HFIR
SNS

Neutron Experiment descriptions:

N1: Triple-Axis Spectrometers, HFIR HB-1A & HB-3
Spin wave and phonon dispersion in Fe-Ga solid solutions

Fe-Ga alloys with appropriate composition and heat treatment, exhibit giant magnetostriction in a polycrystalline and ductile form. The tetragonal magnetostriction coefficient, $\lambda 100$, of Fe-Ga can be up to 15 times that of pure Fe. This makes these materials of tremendous scientific and technological interest for use in devices such as actuators, transducers and sensors. Elastic constant measurements show that the shear elastic constant $1/2(C_{11}-C_{12})$ decreases with increasing gallium concentration and extrapolates to zero at approximately 26 at.% Ga. The slope of the phonon dispersion curve at low-q of the T_2[110] branch is a measure of that elastic constant and hence the interest in measuring phonons in these materials. With the large magnetoelastic interactions in such a material, it is also of interest to measure the spin wave dispersion. The triple-axis spectrometers HB-1, HB-1A and HB-3 will be used to measure both phonon and spin waves of three compositions of Fe-Ga.

N2: Powder Diffractometer, HFIR HB-2A
Magnetic structure of NiO

Neutron diffraction measurements will be performed to investigate the onset of long-range magnetic order in NiO. Data will be collected at various temperatures, ranging from 600K to 288K, using the Neutron Powder Diffractometer at the HFIR. Rietveld analysis of the crystal and low-temperature magnetic structure will be carried out using FullProf Suite software. The results obtained will be discussed and compared with those reported in earlier studies.

N3: Four-Circle Diffractometer, HFIR HB-3A
Structure and lithium-ion motion in the triphylite LiFePO4 studied by single crystal diffraction

Triphylite (LiFePO4) is a promising cathode material for lithium ion batteries due to its virtues of low cost, better safety characteristics, environmental friendliness. But it also faces a significant challenge to achieve both high reversible lithium storage capacity and rapid ion and electron transport capabilities for large-scale EV applications. Studies on the lithium-ion motion properties will help to understand the lithium conduction mechanisms in a lithium ion battery. Using single crystal neutron diffraction, we will resolve the structure of a natural triphylite single crystal at several selected temperatures. Besides the nuclear structure, we are also able to give the magnetic structure at the temperatures lower than its transition temperature. Fullprof and Shelx will be used to refine both nuclear and magnetic structures.

N4: Neutron Imaging Station, HFIR CG-1D
Dynamics of fluid flow in permeable rock

The principle of neutron imaging is based on the attenuation from both absorption and scattering, of a directional neutron beam by the matter through which it passes. Neutron imaging is complementary to other imaging techniques such as X-rays. X-rays are scattered and absorbed by electrons, so absorption and scattering increase monotonically with atomic number. Neutrons, on the other hand, interact with nuclei and their scattering power does not vary in any regular way with atomic number. Several areas of research already benefit from neutron imaging, such as engineering, advanced material characterization, fluid-flow and/or two-phase flow devices, automotive technology, advanced manufacturing technology, applied sciences, aerospace, life and biological sciences, national security applications, etc. Neutrons are specifically well suited for imaging light atoms (hydrocarbons for example) buried in heavy atoms, and are capable of characterizing fluid flow (dynamics). Time resolved water uptake and flow in permeable rocks will be spatially mapped and measured via neutron imaging.

N5: Small Angle Neutron Scattering, HFIR CG-2 General Purpose SANS
HFIR CG-3 Bio-SANS
SNS BL-6 EQ-SANS

Micellar morphologies in self-associated triblock copolymer solutions: effects of concentration and contrast matching in porasils

The PEO-PPO-PEO triblock copolymers have important applications in industry and medicine. Because of the different solubilities of PEO and PPO in water, these copolymers exhibit a rich phase behavior that is sensitive to polymer concentration, solvent ionic strength, temperature, and pressure. These phase changes occur by the self-assembly of the polymer chains into structures with characteristic length scales of the order of few nanometers. Thus, small-angle neutron scattering (SANS) is a technique uniquely well-suited to studying this phase behavior. In these experiments we will study the effects of concentration and ionic strength on block copolymer self-assembly using solutions of 1,2, and 5 wt% Pluronics F108 triblock copolymer in D_2O with varying concentrations of salt added, one series in which the anion is the same and the cation is varied, and another where the reverse is true. The size, morphology, and aggregation number of the micellar structures will be extracted through nonlinear least-squares fitting of the scattering data to model functions.

Contrast-matching SANS has been widely used to characterize structure of soft and biological matter as well as pore accessibility in porous materials. The particular advantage of this technique is attributed to the large difference in coherent scattering lengths of hydrogen and deuterium. By changing composition of protonated and deuterated solvent (such as H_2O and D_2O), one can vary the average scattering length density of the solvent and hence vary the contrast between the scattering objects and surrounding medium. In this experiment, three porasil samples (porous silica) with different H_2O/D_2O ratios (empty pores, i.e. full neutron contrast), pores filled with 71% H_2O + 29% D_2O (intermediate neutron contrast) and 42%H_2O + 58%D_2O (zero-average contrast)) will be measured to demonstrate the power of contrast matching SANS technique.

N6: NOMAD Nanoscale-Ordered Materials Diffractometer, SNS BL-1B
Introduction to Pair Distribution Function analysis

The Nanoscale Ordered Materials Diffractometer (NOMAD) is designed for the determination of pair distribution functions (PDF). The PDF is a measure of the probability to find an atom B at a distance r away from arbitrarily chosen central atom A relative to a random arrangement. As such it is a measure of the atomic arrangement of the sample independent of periodicity and therefore the PDF formalism can be applied equally to liquids, glasses, nanomaterials and long range ordered crystalline materials.
We will determine the PDF of glassy SiO_2 and fit a Continuous Random Network model to it. We will perform an isotope substitution experiment for liquid water. We will look at the PDF of diamond and compare the PDF of bulk and nanocrystalline NiO.

N7: BASIS Backscattering Spectrometer, SNS BL-2
Diffusion dynamics of protons in a novel ionic liquid designed for proton-exchange membranes

Protic ionic liquids show great potential for mobile fuel cell applications. They possess appealing features such as almost negligible vapor pressure, the characteristic electrical conductivity of an ionic conductor, and a sizable temperature gap between the melting and decomposition points. The diffusion dynamics of protons in these complex liquids are closely tied to their performance as electrolytes. Quasielastic neutron scattering (QENS) is a technique of choice for studying the details of diffusion dynamics of hydrogen because of (1) the large incoherent scattering cross-section of hydrogen compared to other elements and (2) capability of probing spatial characteristics of diffusion processes through dependence of the scattering signal on the momentum transfer, Q. The latter is a clear advantage of QENS compared to, for instance, NMR. In our QENS experiment to be performed on the new SNS backscattering spectrometer, BASIS, we will utilize the Q-dependence of the scattering signal to identify and analyze several dynamic processes involving diffusion motions of hydrogen atoms in a recently synthesized ionic liquid [H2NC(dma)2][BETI].

N8: SNAP Spallation Neutrons at Pressure, SNS BL-3
Pressure-induced phase transitions of water at room temperature

Students will load a sample of liquid water into a Paris-Edinburgh pressure cell. They will increase the pressure on the sample first to 1.5 GPa and then to 3 GPa, collecting data at each point. Once analyzed, the data will reveal that the sample has undergone two phase transitions: first from liquid water at ambient pressure to ice VI at 1.5 GPa and second from ice VI to ice VII at 3 GPa.

N9: Magnetism Reflectometer, SNS BL-4A
Revealing magnetism in thin films of normally non-magnetic materials

Understanding the magnetic properties of complex materials near surfaces and interfaces is of critical importance for the development of functional nanostructures and devices. To investigate such structures, where the magnetic layer is only a few unit cells thick and buried within a material, polarized neutron reflectometry is clearly the method-of-choice. During the last two decades Polarized Neutron Reflectometry (PNR) has become a powerful and popular technique in the study of properties of thin films and multilayers. Recent studies show a strong influence of interfaces on the magnetic properties of thin films, leading to behaviors that are radically different from those of bulk materials. Students will apply polarized neutron reflectometry to the study of interfacial magnetism in $LaMnO_3$-thin film epitaxially grown on $SrTiO_3$ substrate. They will mount the sample in the Displex and will learn how to align the sample in the neutron beam of only 50 microns thick. First PNR measurement will be performed at room T. Then the sample will be cooled down to 5K and the measurement will be repeated. The students will process the data using the data reduction programs and will compare the results of the two experiments. With this practice, students will learn polarized neutron reflectometry set-up, in-situ data reduction from 2-D intensity maps, and understand the evolution of properties in thin films with temperature.

N10: Liquids Reflectometer, SNS BL-4B
Polymer self-diffusion studied by specular reflectivity

Isotopic substitution is a powerful tool in neutron scattering studies. In this experiment we will observe the self-diffusion of polystyrene (PS) by means of a 500-Å-thick deuterated (dPS) layer float-deposited atop a spin-coated 500-Å-thick protonated PS layer on a silicon substrate. Students will prepare the film in the beamline 4B wet lab and measure specular reflectivity. We will then anneal the sample for ~30 mins in a vacuum oven and re-measure the reflectivity. Students will fit the data from the two runs to observe changes in the interfacial width of the dPS/PS.

N11: VULCAN Engineering Materials Diffractometer, SNS BL-7
Non-destructive residual stress/strain measurement of weld by neutron diffraction

Residual stresses in engineering component are important to structure lifetime reliability and durability. During welding, severe residual stresses are commonly built up across the weld metal (WM), heat affected zone (HZ) and base metal (BM). The variation of chemical composition and microstructure will also affect the accurate measurement residual stress. Using Time-of-Flight neutron diffraction on VULCAN instrument, the residual stress/strain and the phase distribution can be spatially resolved by engineering diffraction. In the experiment, a weld-bead-on-plate sample will be used for demonstrating the non-destructive residual stress measurement. A stress-free coupon sample, which has similar chemistry of the weld sample, will be used as the reference. Single peak and Rietveld refinement will be used to determine the residual strain and phase concentration of each measurement location, respectively.

N12: POWGEN Powder Diffractometer, SNS BL-11A

Powder Neutron Diffraction for crystal structure refinement and quantitative phase analysis

The student groups will have the opportunity to fill a sample holder with sample powder and perform a helium gas pump-purge of the holder, readying it for neutron diffraction with our FERNS sample changer. They will learn how to set up a run using the Data Acquisition System (DAS) and also reduce data using MantidPlot generating GSAS & Fullprof normalized diffraction data files. Afterwards they will learn Rietveld refinement using Powgen time-of-flight (TOF) neutron diffraction data. Exercises will include

- Sample 1: A simple structure (Ni or LaB_6) to introduce TOF refinement concept.
- Sample 2: Quantitative phase analysis (NIST standard 674b: a mixture of ZnO, TiO2, Cr_2O_3 and CeO_2).
- Sample 3: Finally for those who want to refine a more complex structure, we will look at several models to determine the true crystal structure of Ba_2CuWO_6, which shows a Jahn-Teller distortion.

N13: ARCS Wide-Angular Range Chopper Spectrometer, SNS BL-18

Phonons and spin-waves in the itinerant antiferromagnet $FeGe_2$

$FeGe_2$ is an itinerant antiferromagnet with a Néel temperature of T_N=289 K and a transition to a collinear magnetic structure for temperatures below T=263 K. The magnetic exchange interactions are 15 times stronger along the crystalline c-axis compared to the a and b axes. We will be using the ARCS instrument to measure the lattice and magnetic excitations in $FeGe_2$ for temperatures above and below the Néel temperature. We will be measuring large regions of reciprocal space in order to extract the phonon and spin-wave dispersion relations.