Neutron Experiments descriptions:

N1. Triple-axis Spectrometers: HB-1A, HB-1, HB-3

"Spin wave and phonon dispersion in Fe-Ga solid solutions"
Jerel Zarestky, Masaaki Matsuda, Mark Lumsden

Fe-Ga alloys with appropriate composition and heat treatment, exhibit giant magnetostriction in a polycrystalline and ductile form. The tetragonal magnetostriction coefficient, λ_{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 $1/2(C_{11}\text{-}C_{12})$ 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, HB1, HB-1A, & HB-3, will be used to measure both phonon and spin waves of three compositions of Fe-Ga .

N2. Wide Angle Neutron Diffraction: HB-2C

"Time-resolved Hydration of Portland Cement Monitored by Neutron Powder Diffraction"
Bryan Chakoumakos

The phase evaluation in ordinary Portland cement pre-mixed with heavy water will be monitored in situ by neutron diffraction patterns using the WAND instrument at the HFIR. The high flux of the WAND and PSD detector enable rapid data collection. Repeated data collections (in minutes) will be recorded over several hours. Modeling the phase evolution will be done with Fullprof software suite.

N3. Quasi-Elastic Neutron Scattering - BASIS: BL-2

"Diffusion dynamics of protons in a novel ionic liquid designed for proton-exchange membranes"
Eugene Mamontov

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].

N4. Liquids Reflectometer (horizontal surface): BL-4B

"Polymer self-diffusion studied by specular reflectivity"
John Ankner

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.

N5. General-Purpose Small Angle Neutron Scattering: CG-2

"*Micellar Morphologies in Self-Associated Triblock Copolymer Solutions"*
Ken Littrell

The PEO-PPO-PEO triblock copolymers have important applications in industry and medicine. Because of the differing 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 most appropriately measured in nanometers. Thus, small-angle neutron scattering (SANS) is a probe uniquely well-suited to studying this phase behavior. In these experiments we will probe the effects of concentration and ionic strength on block copolymer self-assembly using solutions of 1,2, and 5 weight% Pluronics F108 triblock copolymer in D20 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.

N6. Bio-SANS: CG-3

"Protein unfolding studied by small-angle neutron scattering"
Volker Urban

Small-angle neutron scattering (SANS) is a powerful tool for looking at the conformation of biological macromolecules in solution. SANS is particularly sensitive to conformational changes of proteins and nucleic acids in response to applied stimuli, such as temperature, pressure or small molecules. We will study the solution conformation of human serum albumin, a multifunction protein found in the blood, and how it changes in response to urea, a protein denaturant, using the BioSANS instrument at HFIR. Various methods of fitting the data will be employed to extract the molecular weight of the scattering particle, the radius of gyration, the distance distribution function P(r) and the maximum linear dimension. Methods for developing models of the protein from SANS data will also be discussed.

N7. Neutron Powder Diffraction: HB-2A

"Magnetic structure of NiO"
Vasile Garlea

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.

N8. Engineering Materials Diffractometer (VULCAN): BL-7

"In-situ neutron diffraction measurement of intergranular strain evolution in 316 stainless steel under uniaxial loading at VULCAN"
Ke An

Anisotropic materials such as stainless steels will develop strong intergranular strains in the regime of plastic deformation. Neutron diffraction allows strain/stress measurement at depth by its high penetration through most engineering materials. The lattice strains of different lattice plane can be calculated by Bragg peak shift with respect to zero strain/stress a reference. At spallation neutron source, using time-of-flight materials science and engineering diffractomter VULCAN can probe changes of lattice strain of all possible hkl directions under in-situ loading. In this experiment, a cubic fcc stainless steel dog bone sample of 6mm in diameter will be applied tensile loading continuously up to 5% engineering strain by using the VULCAN MTS loadframe, in the meantime neutron diffraction pattern of the steel sample will be collected. The neutron data will be separated and reduced based on the load intervals. Single peak refinement will be used for analyzing the intergranular strains of [111], [200], [220] and [311] lattice plane in the material under uniaxial loading. Through this practice, students will learn in-situ loading neutron diffraction measurement set-up at materials science and engineering diffractomter VULCAN ; lattice strain data calculation from diffraction pattern using VDRIVE software, and understand the nature of intergranular strain evolution of material under loading..

N9. Spallation Neutrons and Pressure Diffractometer (SNAP): BL-3

"Pressure-induced phase transitions of water at room temperature"
Chris Tulk

Students will load a sample of liquid water into a Paris-Edinburgh pressure cell. They'll 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.

N10. Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA): BL-17

"Dynamics of metal hydride systems: Harmonic oscillators and beyond"
Garrett Granroth

The hydrogen in zirconium hydride (ZrH_2) sits at the interstitial positions between the zirconium. At the simplest description, the energy levels can be considered to be the same as a particle in a potential well. The aim of this experiment is to measure the vibrational spectrum of ZrH2 as a function of energy and wavevector transfer, and determine how well it conforms to the predictions of the scattering from a harmonic oscillator. Practical applications of sample preparation, data collection and analysis will be given to generate the scattering function $S(Q,\omega)$ from the data. This will be compared to theoretical predictions based on the harmonic oscillator description, with a discussion of what may cause any discrepancies found. As time permits, other metal hydrides will be measured to highlight differences in their energy spectra.