2024 Neutron Tutorial Descriptions

Group 1 (N1-N3): Inelastic Neutron Scattering

N1: HB-1A and HB-3 Triple-Axis Spectrometers, HFIR

Spin wave and phonon dispersion in Fe-Ga solid solutions

Triple axis spectroscopy (TAS) is a versatile technique for measuring the scattering function in energy and momentum space. These measurements allow one to probe the static and dynamic properties of a wide range of materials. The TAS team will demonstrate how to carry out a TAS experiment. This tutorial will cover single crystal sample alignment and how to set up typical elastic and inelastic scans in SPICE (Spectrometer Instrument Control Environment), using Fa-Ga alloy single crystal samples as an example. These materials exhibit giant magnetostriction and are of tremendous scientific and technological interest for use in devices such as actuators, transducers, and sensors.

N2: HYSPEC Hybrid Spectrometer, SNS

Separating nuclear and magnetic scattering using neutron polarization analysis

Polarized neutron measurements unambiguously distinguish between structural and magnetic scattering features, allowing us to determine the direction of magnetic moments and their fluctuations. By employing polarization filters, magnetic guide fields, and 'spin flippers,' we selectively choose neutrons of a specific orientation. At HYSPEC, two distinct modes of running polarized experiments exist: a "half-polarized" mode where successive measurements with polarized incident beam oriented parallel and anti-parallel to the external magnetic field are performed without polarization analysis of the scattered beam, or a "XYZ-polarization analysis" where neutron spin flip effects are measured by analyzing the final polarization with respect to the incoming polarization. XYZ refers to the ability to reorient the guide field at the sample position in orthogonal directions using an array of electromagnetic coils. In this exercise we demonstrate XYZ-polarization analysis to separate nuclear coherent, nuclear spin-incoherent, and magnetic scattering for standard materials (Fe, TiZr, V-rods, and MnO powder sample). This exercise enhances students' understanding of polarized neutron scattering and provides experience with data processing and visualization using the MSlice package.

N3: SEQUOIA Fine-Resolution Fermi Chopper Spectrometer, SNS

Dynamics of metal hydride systems: Harmonic oscillators and beyond

The hydrogen in zirconium hydride (ZrH2) sits at the interstitial positions between the zirconium. At the simplest description, the energy levels are the same as a particle in a potential well. The aim of this experiment is to measure the vibrational spectrum of ZrH_2 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. As time permits, other metal hydrides will be measured to highlight differences in their energy spectra.

Group 2 (N4-N6): Chemical Spectroscopy

N4: BASIS Backscattering Spectrometer, SNS

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 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 synthesized ionic liquid $[H_2NC(dma)_2][BETI]$.

N5: VISION Vibrational Spectrometer, SNS

Proton dynamics in phosphoric acid

Phosphoric acid, H_3PO_4, is a tribasic acid commercially available an 85% aqueous solution. The annual production of phosphoric acid is in the tens of megatons range. It is used mainly in the production of fertilizers, but also in the food and cleaning agents industry. In its anhydrous form it crystallizes as a monoclinic solid with a complex network of hydrogen bonds. We will use VISION to examine proton dynamics phosphoric acid. Use will be made of the diffraction detector on the beam line, which permits the simultaneous collection of diffraction and inelastic data. VISION has a dedicated computer cluster for data analysis. In parallel with the experiment, we will calculate the vibrational spectrum of phosphoric acid with Density Functional Theory (DFT) to show how these calculations support spectral interpretation. Use of the new software, O'climax to convert computed vibrational modes to a density of vibrational states directly comparable with VISION data will be demonstrated.

N6: NSE Neutron Spin Echo Spectrometer, SNS

Dynamics of Surfactant Micelles

We will investigate the dynamics of sodium dodecyl sulfate (SDS) micelles. The goal of the experiment is to measure the effective diffusion coefficient of the SDS micelles suspended in heavy water. This "classic" NSE experiment will allow us to illustrate the basic principles of the NSE technique and the required measurements and corrections. We will go through the reduction process starting from raw data to the intermediate scattering function. Finally, by comparing the results with model calculations, we will show the link between the structure and the dynamics in colloidal fluids.

Group 3 (N7-N10): Neutron Powder Diffraction

N7: HB-2A Powder Diffractometer, HFIR

Solving the magnetic structure of a chiral symmetry spin Ising system

The POWDER neutron diffractometer is an instrument optimized for studying complex magnetic systems under a wide variety of sample environment conditions (e.g. temperatures from 0.03 to 1800 K, magnetic fields up to 8 T and pressures up to 2 GPa). In this demonstration we will start with a tour of the beamline, describing its components, demonstrating its operation, and discussing the available sample environments. We will then look at data collected on the chiral pyrogermanate $Er_2Ge_2O_7$ at ultra-low temperatures and under an applied magnetic field. A low temperature antiferromagnetic transition will be identified, and Rietveld refinements will be performed to model both the nuclear and magnetic scattering. To solve the magnetic structure, students will be shown how to determine a magnetic ordering vector in a powder sample and then introduced to the tools of representational analysis to generate possible magnetic structures and come to a best fit model. The solution will be discussed within the context of the physics of the system and the implications of the solved structure for the magnetic spin-Hamiltonian will be considered.

N8: HIDRA Engineering Materials Diffractometer, HFIR

Non-destructive residual stress/strain measurement of machined aluminum bar

"Engineering Diffractometers" are neutron diffractometers with fine collimation of the incident and diffracted beams which can be used to obtain diffraction patterns from small well-defined volumes inside bulk materials. The diffraction pattern can be analyzed to identify and quantify the crystalline phases present, the degree of preferred orientation, and deviations from the stress-free lattice parameters (i.e., strain), which indicate residual stress. Residual stresses in engineering components are important to structure lifetime, reliability and durability. Mechanical processing, extrusion, bending, forging, and joining of metals all can result in significant residual stress in engineering components, and these stresses directly impact service life.

This project will focus on how engineering diffractometers at both a spallation source (VULCAN) and a reactor source (HIDRA) have unique advantages which can be used to characterize complex materials using a sample containing residual stress. A token sample has been prepared whereby a measurement of residual stress via neutron diffraction can be compared to other destructive techniques such as the contour method. The residual stress in the part will be mapped and the results compared and experimental considerations for measurements will be discussed. The students will gain an understanding of how to plan and execute a successful diffraction experiment on HIDRA as well how to analyze data observed during a typical experiment.

N9: NOMAD Nanoscale-Ordered Materials Diffractometer, SNS

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 $BaTi_2O_5$. We will introduce real-space fitting using the 'small-box' refinement program PDFgui, modeling the PDF of diamond, crystalline SnO_2, and SnO_2 nanoparticles.

N10: POWGEN Powder Diffractometer, SNS

Powder Neutron Diffraction for crystal structure refinement and quantitative phase analysis

The student groups will have the opportunity to learn how 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 POWGEN Automatic Changer (PAC) sample changer. They will learn how to set up a run using the Data Acquisition System (DAS). Afterwards they will learn Rietveld refinement on Powgen time-of-flight (TOF) neutron diffraction data using GSAS-II. Exercises will include

- Sample 1: A simple structure (LaB_6) to introduce TOF refinement concept.
- Sample 2: Quantitative phase analysis (NIST standard 674b: a mixture of ZnO, TiO_2, Cr_2O_3 and CeO_2).
- Sample 3: Refine magnetic structure of Quasi-One-Dimensional van der Waals CrSbSe3
  Sample 4: Finally, those who get through the first three examples will be able to learn to refine a more complex structure. We will look at two models to determine the true crystal structure of Ba_2CuWO_6, which shows a Jahn-Teller distortion.

Group 4 (N11-N14): Neutron Single Crystal Diffraction

N11: WAND^2 Wide-angle Neutron Diffractometer, HFIR

Crystallographic superstructures in Pr_2PdSi_3

The intermetallic compound series R_2PdSi_3 (R = rare earth metal) exhibits some interesting magnetic properties as giant magneto-resistance effect, strong anisotropy in the electronic properties and a generic field induced phase. The magnetic structures are quite complex with large magnetic unit cells due to the delicate interplay between competing crystal electric field effect and magnetic exchange interaction and the addition of geometric frustration. The hexagonal crystallographic structure is formed from the sequence of triangular rare earth layers and Pd/Si layers stacked along the c-axis. The Pd/Si layers obey site occupation rules of its ions and the stacking of the layers yields a crystallographic superstructure. WAND² has a 2D-position sensitive detector covering 120° in-plane and 15° out-of plane. By rotating the sample, a huge area of reciprocal space is mapped. The high efficiency and low background of the instrument allows the detection of very weak reflections. Using the remote control, the sample will be aligned and a scan for a full reciprocal map setup. The data will be reduced and analyzed using MantidWorkbench and FullProf.

N12: DEMAND Single Crystal Diffractometer, HFIR

Structure and lithium-ion motion in the triphylite $LiFePO_4$ studied by single crystal diffraction

Triphylite, $Li(Fe,Mn)PO_4$, is a candidate cathode material for lithium ion batteries due to its virtues of low cost, better safety characteristics and 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. Unrelated, this solid solution also exhibits antiferromagnetism at low temperatures. Using single crystal neutron diffraction, one can refine the nuclear structure (atom positions, anisotropic atomic displacement parameters, Fe/Mn ratio, Li content) and the magnetic structure (Fe/Mn moment magnitudes). Data sets, exercises and user guides will be provided to refine both nuclear and magnetic structures using Fullprof.

N13: CORELLI Elastic Diffuse Scattering Spectrometer, SNS

Introduction to diffuse scattering analysis based on single crystal measurement

CORELLI is a statistical chopper spectrometer with energy discrimination located at beam-line 9 at the SNS. CORELLI is designed and optimized to probe short-range correlation of crystalline materials through single-crystal diffraction and elastic diffuse scattering. CORELLI combines the high efficiency of white-beam Laue diffraction with energy discrimination by modulating the beam with a unique statistical chopper. We will practice the experimental setup, data collection, data reduction on a single crystal of Bixybite $(Mn_{1-x}Fe_x)_2O_3$. Data collection strategy will be optimized based on initial sample orientation determination. Data reduction and visualization (including the comparison of total and elastic-only spectrum) will be performed using Mantid. The normalized data will be used to perform three dimensional (3D)-PDF using the punch-fill method to reveal the short-range correlation in the system.

N14: TOPAZ Single Crystal Diffractometer, SNS

High-resolution single crystal structure analysis using wavelength-resolved Laue diffraction

TOPAZ is a high-resolution single crystal diffractometer for the study of nuclear and magnetic structures of materials at sub-atomic resolution. It uses a large array of neutron time-of-flight detectors for data collection in wavelength-resolved Laue mode to cover a large 3D volume of reciprocal space, or Q-space (after unit conversion from neutron events recorded in detector x, y and a band of neutron wavelengths). We will practice the experimental setup, data collection, data reduction and perform a structure refinement

of a single crystal dataset of scolecite ($CaAl_2Si_3O_{10}\cdot 3H_2O$) measured on TOPAZ to locate the missing hydrogen atoms on the water molecules. Scolecite is the calcium member of the natrolite family within the zeolite group. The cation and hydrogen bonding interaction of the water molecules with the framework plays an important role in fine-tuning the adsorption and electrostatic properties of the porous zeolite channels, which is fundamental for applications in separation science and energy storage materials. Single crystal data collection strategy will be optimized with the CrystalPlan program. Peak integration will be performed in 3D Q-space in Mantid. Data reduction including neutron TOF spectrum, detector efficiency, and absorption corrections will be carried out with the TOPAZ ReductionGUI. The structure will be refined using JANA2020. The option to refine the neutron structure in SHELXL, JANA2020 and Olex2 will also be explored.

Group 5 (N15): Neutron Imaging

N15: MARS Multimodal Advanced Radiography Station, HFIR, and VENUS Versatile Neutron Imaging Instrument, SNS

Seeing the inside

Given the unique interactions of neutrons with materials, neutron imaging is a complementary technique to X-ray imaging that can spatially resolve internal features/distributions non-destructively in bulk systems. Neutrons' high sensitivity to light elements such as H and Li enables the ability to visualize the water transport in plant roots or the Li transport in an operating battery. By participating in this experiment, you will gain the experience of running a neutron imaging experiment, including 2D radiographs and 3D tomography, and performing data analysis on a materials science sample. Additionally, you will be able to tour the SNS's upcoming Versatile Neutron Imaging Instrument (VENUS) that focuses on time-of-flight imaging to make use of neutron scattering Bragg features for improved contrast and phase identification and is poised to join the user program in 2025. Students will learn how to process and fit Bragg edges of crystalline powders using in-house software iBeatles. They will also learn about how the imaging team has developed an autonomous hyperspectral computed tomography capability using machine learning.

Group 6 (N16-N19): Small-Angle Neutron Scattering

N16: GP-SANS General Purpose Small Angle Neutron Scattering, HFIR

A contrast matching study of porous silica using small-angle neutron scattering

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 (i.e. varying the volume fraction of H_2O in the mixture of H2O and D_2O), one can change the average scattering length density of the solvent and hence vary the contrast between the scattering objects and surrounding medium. In this experiment, six porasil samples (porous silica) with different H_2O volume fractions (0%, 20%, 40%, 60%, 80% and empty porasil sample) will be measured. Model-independent data analysis will provide information on porosity, specific surface area as well as contrast matching point to get average scattering length density of the material. Model-dependent data analysis will provide information on the pore diameter and pore-pore distance.

N17: Magnetic SANS at GP-SANS, HFIR

Probing magnetic diffraction using Small Angle Neutron Scattering.

Neutron scattering is a powerful technique for investigating material characteristics. By using the properties of a neutron such as the fact that the neutron has spin-- making it sensitive to changes in magnetic

states and structures-- one can probe magnetic properties of a whole host of materials. Small-angle Neutron Scattering (SANS) is a technique used to study large-scale structures varying from 1 to 500 nanometers. We will be preforming an experiment on single crystal of niobium that is a Type II superconductor. This sample has a clear magnetic diffraction pattern that we will use to show how magnetic diffraction data is collected and analyzed on GP-SANS.

N18: Bio-SANS Biological Small-Angle Neutron Scattering, HFIR

Methods for interpreting biological small-angle neutron scattering data

Contrast-matching SANS is widely used to characterize a wide variety of soft and biological matter systems. The large difference in coherent scattering lengths of hydrogen and deuterium nuclei enables unique measurements that are not possible by other techniques. By varying the composition between fully protonated and fully deuterated solvents (such as H_2O and D_2O), one can vary the average scattering length density of the solvent and hence alter the contrast between the individual components in a complex system and surrounding medium. To demonstrate the strength of contrast variation, in this experiment, we will measure maltose-binding protein (MBP) dissolved in a series of H_2O/D_2O solvent ratios (0 – 100%) to illustrate how changing the contrast between MBP and the solvent impacts the scattering signal. We will employ different analysis approaches that can be applied to the SANS data, including simple methods like Guinier Analysis for determining radius of gyration and Kratky plots for protein flexibility. Using contrast variation data of MBP, we will identify the solvent condition that achieves contrast matching, completely masking the protein signal. For more advanced analysis, we will employ ab initio methods using the ATSAS package to obtain solution structures of the protein, such as the dummy atom model or ensemble of models, and investigate how its solution structure compares to its crystal structure.

N19: EQ-SANS Extended Q-Range Small-Angle Neutron Scattering, SNS

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 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.

Group 7 (N20-N21): Neutron Reflectometry

N20: MAGREF Magnetism Reflectometer, SNS

Revealing magnetism in thin films of normally non-magnetic materials

Understanding the magnetic properties of complex materials near surfaces and interfaces critically important 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. Polarized Neutron Reflectometry (PNR) is a powerful 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 study interfacial magnetism in a $LaMnO_3$-thin film epitaxially grown on a $SrTiO_3$ substrate. The sample will be mounted in the closed cycle refrigerator and students 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 to 5K and the measurement will be repeated. The students will learn how to process the data using the data reduction program 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.

N21: LIQREF Liquids Reflectometer, SNS

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 [1]. Students will prepare the film in the beamline 4B wet lab and measure specular reflectivity. We will then anneal the sample for ~30 min 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.

1. A. Karim, et al., *Short-time relaxation and polymeric interfaces.* Physical Review B **42,** 6846 (1990).

Group 8 (N22-N25): Complex Sample Environments

N22: VULCAN Engineering Materials Diffractometer, SNS

Lattice strain determination of intergranular strain and phase transformation evolution in stainless steel under uniaxial loading

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, and the strain induced phase transformation facilitates both work hardening and ductility of the material. At the Spallation Neutron Source, VULCAN can probe changes of lattice strain of all possible *hkl* directions and monitor the phase transformation under in-situ loading. This practical will focus heavily on the complex data analysis, specifically on lattice strain data calculation from diffraction pattern using VDRIVE software. 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 planes in the material and Rietveld refinement will be used for phase analysis. The students will also have the opportunity to see the VULCAN instrument and its unique set-ups for strain measurements including dedicated load frames. Through this the students will

understand the nature of intergranular strain evolution and strain induced phase transformation of material under loading.

N23: High Temperature Group, SNS Sample Environment

Sample preparation, planning, and operation of high temperature vacuum furnaces

The Sample Environment (SE) group in neutron sciences at ORNL operates several different high-temperature devices, ranging from room temperature up to over 2000^{o} C, in support of neutron scattering experiments. For this experiment, students will learn how the different furnaces operate and gain knowledge on the different internal components of the furnaces. Students will have the opportunity to see a conventional furnace that is disassembled, and to assemble some main components of the systems in a hands-on exercise. Students will learn what proper materials are used for sample holders at high temperature. The students will be presented with the different types of heating that the equipment provides, such as radiative vs. conductive, and what the effects are on the sample in terms of temperature gradients and homogeneity. The students will learn how to properly mount samples onto the sample sticks, using good mechanical and vacuum practices, and how to determine the sample position inside of the equipment to ensure alignment of the sample in the neutron beam. Additionally, students will learn how different levitation techniques are possible, and which ones are currently implemented at the SNS. Students will be able to experience the sample preparation process, the mechanical mechanisms, and operation of an aerodynamic levitator. Experiments at high temperature require special considerations for sample preparation, operation, and safety; the discussion of how to coordinate with sample environment and beamline staff to prepare for these experiments from the proposal stage through beamtime will follow.

N24: RheoSANS – Rheology and Small-Angle Neutron Scattering, Shull Wollan Center

Nanoscale Structures of Colloidal Dispersions under Shear

Rheology is the science of flow and deformation of matter. The rheological properties of colloidal systems are controlled by the sizes, shapes, and interactions of dissolved species. Rheo-SANS studies the structure of matter exposed to shear in-situ, and can provide detailed, nanoscale insights into the properties of colloidal systems. For liquid samples, the Couette geometry is often used in rheo-SANS experiments, allowing structural studies in the flow-vorticity plane is probed in radial configuration, and the velocity gradient – vorticity plane is probed in tangential configuration. Careful analysis of these scattering data in combination with rheology data allows to unravel the microscopic origins of shear thinning, and continuous and discontinuous shear thickening. In this tutorial, a brief introduction into rheology measurements and rheo-SANS will be given. We will then study two systems with complex rheologies using rheo-SANS: Stober silica particle dispersions, and polymeric micelle solutions. Rheo-SANS measurements in different shear planes will be analyzed to understand the complex 3D structures of these systems under shear.

N25: Resonant Ultrasound Spectroscopy, SNS Sample Environment

In situ Resonant Ultrasound Spectroscopy probe for Neutron Scattering

As an example of new "multimodal" experimental capabilities, this practice involves measurement and data analysis with the new *in situ* Resonant Ultrasound Spectroscopy (RUS) probe.

RUS is being integrated with low and high temperature sample environment to expand the options for in-situ characterization of materials during neutron scattering experiments. The RUS technique provides high-precision, non-destructive, neutron-scattering-compatible measurements of the elastic constants and sound-attenuation in materials. In addition, the ultrasonic response in the vicinity of phase transitions enables a high-precision tracking of the sample state in-situ, more precisely than through temperature or magnetic field sensors.

The students will learn how to perform measurements of elastic moduli exploring the sensitivity of the probe with small changes of temperature and to calculate elastic moduli from measured resonance modes.

Group 9: Neutron Data Science (N26)

N26: Data Science for Neutron Scattering, SNS

Data science permeates the field of neutron scattering at all levels, from controlling instrumentation on the beamline, through data reduction and into data analysis. This tutorial targets beginner-to-intermediate level and aims to provide an *interactive* introduction to some of the cornerstones of data science including:

- Creating and managing repositories using git and accessing code and collaborating with GitHub
- What is conda (and why is it important)?
- An overview of the vast landscape of useful tools (and how to import these into your own code)
- An introduction to python scripting for neutron science

After this introduction, we will offer a series of parallel interactive tutorials to cover a range of abilities. These tutorials will focus on some specific applications in the field of neutron scattering (such as the mantid framework), as well as some more general themes (for example, fitting data).