National School of Neutron and X-ray Scattering
Neutron Scattering Experiments 2007

Neutron Experiment Coordinator: Alexander Kolesnikov

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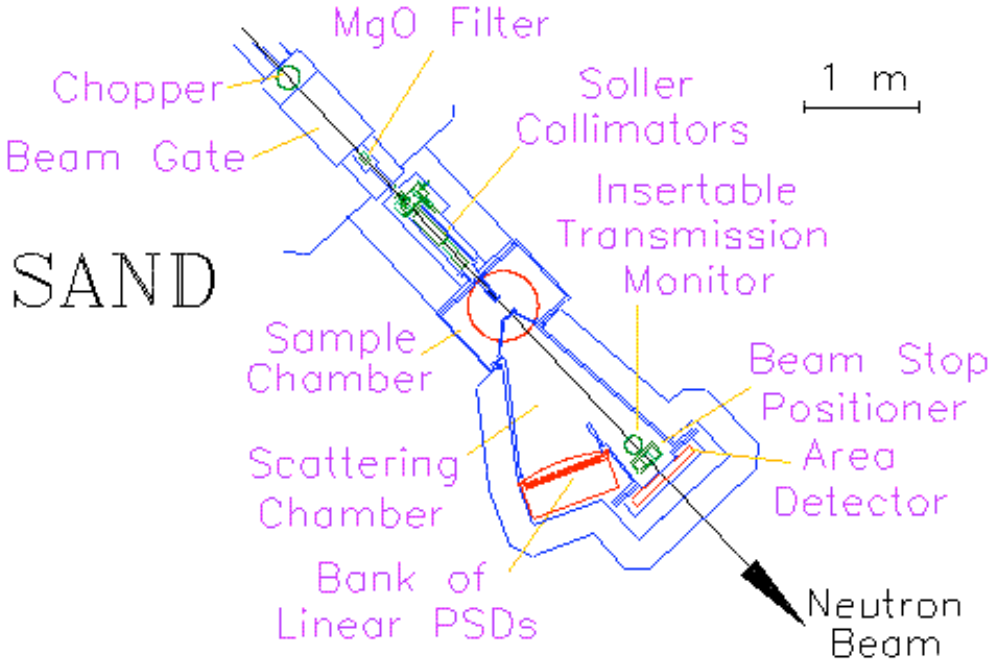
N1: Small Angle Neutron Scattering
"Micellar phenomena in aqueous triblock copolymer solutions".

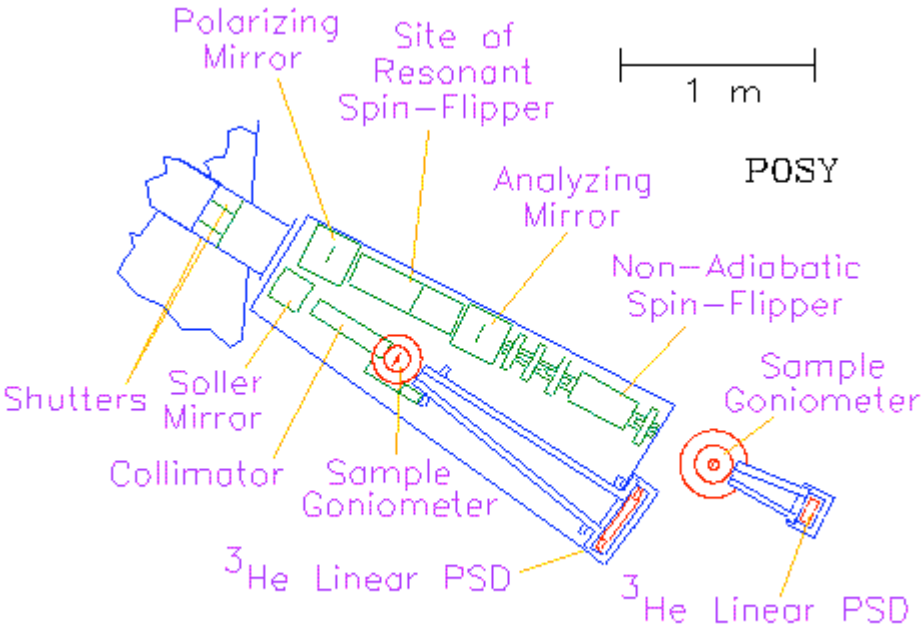
Description: The micellar phase behavior of surfactant systems is highly important in medicine and industry. Due to the difference in the hydrophobicity of the two polymer segments - PEO and PPO, the aqueous PEO-PPO-PEO triblock copolymers in aqueous media exhibit a rich micellar phase behavior with a variety of different morphologies depending on the polymer concentration, chain length, temperature and salt concentration. SANS is a high sensitivity probe to learn about the size and shape of particles with length scales in the range of 1 to 100 nm. In this experiment we will introduce the features of the SANS instruments at the steady state and pulsed sources, the methodology to use the pulsed source based SAND instrument at the IPNS and derive the structural features such as size, shape, aggregation number, volume fraction of the micelles from the SANS data of block copolymer solutions as a function of temperature and salt concentration.



Instrument – SAND
Instructors - Venky Pingali and P. Thiyagarajan

N2: Neutron reflectivity
"Polymer films on silicon wafer".

Description: Neutron reflectivity is an excellent tool for learning about the depth dependent characteristics of a film. In this experiment you will investigate these characteristics of a spin coated polymer film using the neutron reflectometer POSYII at IPNS. You will learn the technical aspects of performing a measurement on the instrument, such as mounting, properly aligning and understanding the raw data as it is collected. Data processing programs, which let you convert the raw data to a reflectivity curve, will be covered, as well as learning what conclusions can be drawn by looking at this curve, even before the final step of fitting the data. Additionally, on POSY1 you will see how using polarized neutrons one becomes sensitive to the magnetism of a sample. Finally you will learn how understanding reflectivity is important in the design of new neutron scattering instrumentation, such as at SNS, by performing Monte Carlo simulations.



POSY II

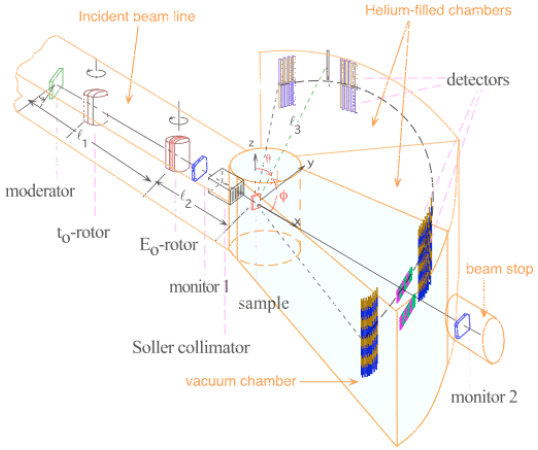
Instrument - POSY I/ POSYII
Instructors - Suzanne G.E. te Velthuis, Ursula Perez-Salas

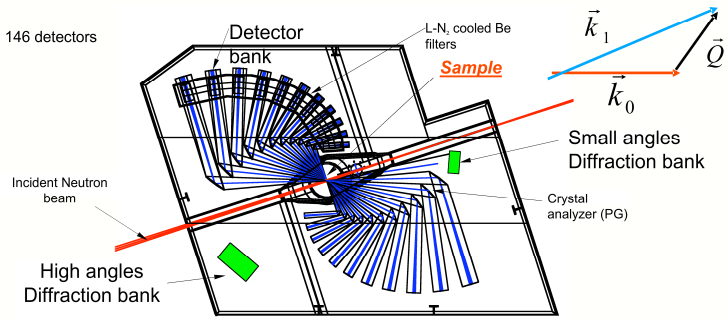
N3: Inelastic and Quasielastic Neutron Scattering
"Neutron Spectroscopy of molecular crystals"

Description: HRMECS is a direct geometry time-of-flight spectrometer used for inelastic neutron scattering study of the vibrational dynamics for different materials in wide range of neutron energy (0.5-800 meV) and momentum (0.2-30 Å-1) transfers. Using the example of aluminum trihydride students will do a virtual inelastic neutron scattering experiment. Then they will use the experimental data from the previous Neutron School, lean how to reduce the raw data to obtain the dynamical structure factor S(Q,E) and generalized density of phonon states G(E) for AlH3. The analysis will include the separation of single-phonon and multiphonon contributions to the spectra as well as a determination of the mean-squared displacement of the hydrogen atoms.

QENS is a "crystal-analyzer" or "inverse-geometry" neutron spectrometer that accepts a white beam from the solid methane moderator onto the sample. This efficient use of neutrons allows for dynamical studies, *viz.* chemical spectroscopy at low energies and quasi-elastic scattering from diffusive motions, also when the amount of sample in the beam is necessarily very small. Examples of QENS studies include the dynamics of small molecules adsorbed in systems such as zeolites, clays, and intercalated graphite, and of chemical samples which cannot be made in large quantities. The students will learn how to reduce and analyze QENS data illustrating the rotational tunneling of molecular hydrogen, the glass transition in polymeric materials, and the molecular dynamics of bulk liquid water.

HRMECS **QENS**



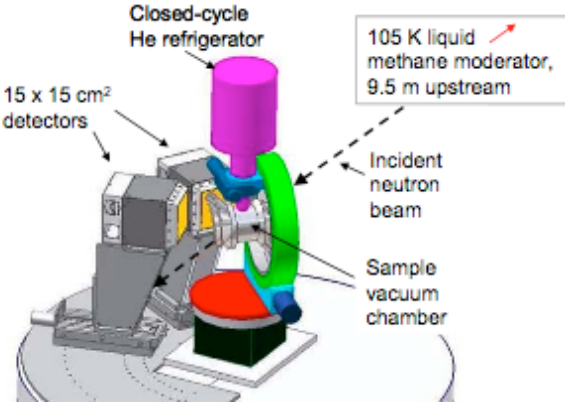


Instruments - HRMECS and QENS
Instructors - Alexander Kolesnikov and Nicolas de Souza

N4: Single Crystal Neutron Diffraction
"Single Crystal Neutron Diffraction: SCD."

Description: Both scientific and practical explanations of neutron crystallography at a time-of-flight source will be covered, single crystal analysis works, and how it will be applied to data collected on the IPNS Single Crystal Diffractometer (SCD). The students will tour the SCD and data from oxalic acid dihydrate and partially deuterated $(NH_4)_2[Cu(H_2O)_6](SO_4)_2$ will be analyzed to characterize hydrogen bonds and to determine the degree of deuteration.

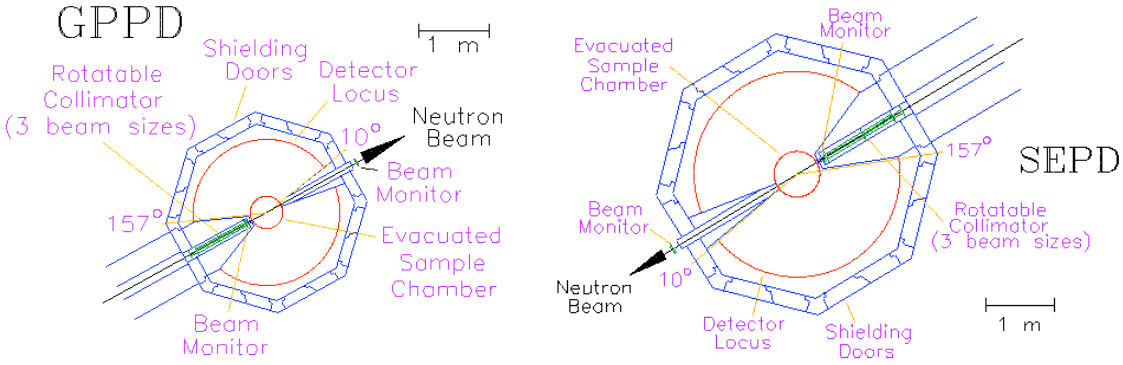
SCD



Instruments –SCD
Instructor –Art Schultz

N4: Neutron Powder Diffraction
"Neutron Powder Diffraction: SEPD and GPPD."

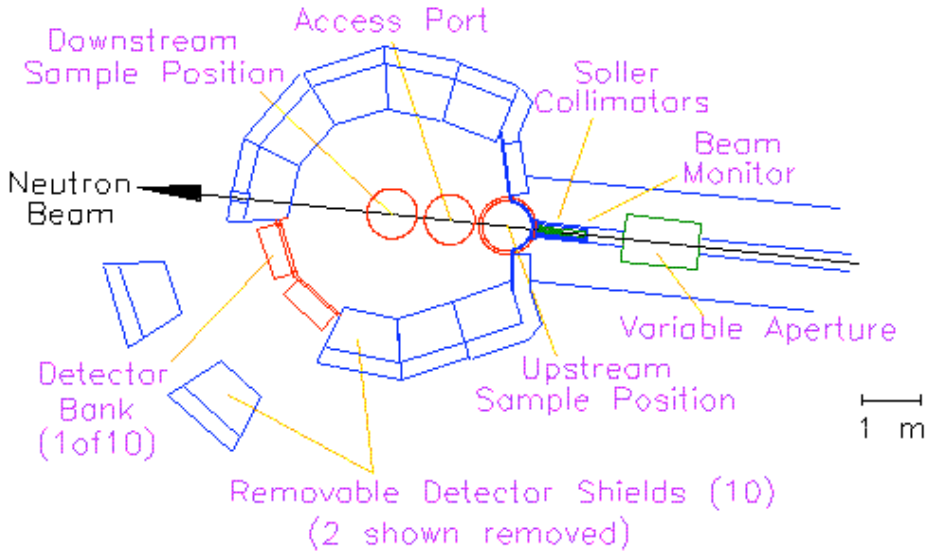
Description: Both scientific and practical explanations of the neutron diffractometers will be covered, including how the GSAS Rietveld powder analysis works, and how it will be applied to data collected on the instruments. Experimental operation will be shown on both the SEPD and GPPD instruments. The students will get a tour of the two instruments and members of each group will pack one sample and put it on the changer, thus seeing the inside of the instrument. Y_2O_3 is a relatively standard material and will be used to introduce the concepts of Rietveld analysis. More complex experiments will focus on two perovskites. The data files will be available on the CD each student will receive. Finally a more challenging set of samples will be run on each instrument and given to the students to analyze.



Instruments – SEPD and GPPD
Instructors – Jim Richardson and Bob von Dreele

N6: Liquid Scattering
"The structure of glasses and liquids."

Description: A short course centered around neutron experiments on the Glass Liquid and Amorphous materials Diffractometer has been designed to demonstrate the fundamental principles of liquid and glass structure determination. The technique of pulsed neutron diffraction using total and isotopic substitution is explained, together with the concept of radial distribution functions, coordination numbers and intermediate range ordering. Measurements on water and vitreous silica are used as examples. The advantages of combining complimentary neutron and high energy x-ray data are described for the case of germania and current trends in computer modeling techniques of diffraction data are briefly reviewed. Experiments will be taken from current research examples of the GLAD group at IPNS and collaborators. In previous schools, GLAD experiments have had a fundamental scientific bias related to the phenomenon of 'polyamorphism' or the structure/property relationship in rare earth aluminate glasses for use in optical and laser applications.



Instrument - GLAD
Instructors - Chris Benmore, Joerg Neuefeind (SNS), Joan Siewenie and Qiang Mei.