The recently installed (July 2003) Advanced Neutron Diffractometer/Reflectometer (AND/R) adds new capabilities for bio-membrane research and diffuse scattering measurement to the NCNR. It aims to provide a focal point for structural biology research, combining an increased in-house staff to serve and interact with an expanded user program. Furthermore, it will benefit the NCNR reflectometry program by increasing available beam time overall. Of the AND/R beamtime, 75% will be available to the CNBT partners and 25% to general users through the NCNR proposal system. With the AND/R located just upstream of NG-1 reflectometer, this pair of instruments will share common facilities, equipment, and expertise.

The AND/R is the centerpiece of the Cold Neutrons for Biology and Technology (CNBT) program, which is committed to the development of advanced neutron scattering instruments for studies of membrane systems. CNBT was funded by the National Institutes of Health (NIH), National Center for Research Resources on September 2001 with additional support from NIST, the University of California at Irvine and the University of Pennsylvania. The CNBT partnership consists of investigators from six universities: UC Irvine (principal investigator Stephen H. White), Johns Hopkins University, Penn, Rice, Duke, Carnegie Mellon and investigators from NIST. Additional collaborators are from UC San Diego, Los Alamos National Laboratory, and the NIH. The facilities consist of the AND/R, a 30 m small-angle neutron spectrometer (SANS) dedicated 10% to CNBT, a fully equipped biology laboratory, and two state-of-the-art computer facilities (one at U C Irvine, and one at NCNR) for molecular dynamics computations. This combination provides a new capability for the United States.

The AND/R is modeled after the highly successful polarized beam reflectometer on the NG-1 neutron guide. Like the NG-1 reflectometer, the AND/R will have a horizontal scattering plane, which provides unrestricted access to higher scattering angles. Other features common to both instruments are the polarized beam capability to enable the use of magnetic reference layers for phase inversion of data, and a vertically focusing monochromator to increase the flux on the sample.

Additional features make the instrument well suited for both reflectometry and diffraction investigations of biological systems. First, the AND/R can operate using either a larger 5 cm “pencil” detector (increasing the flux at higher momentum transfer, $Q$) or a 2-dimensional position sensitive detector (PSD). By simultaneously measuring non-specular scattering from large areas in reciprocal space, the PSD will make it much more efficient to obtain information on in-plane structures. Also, the sample tables will accommodate larger sample environments (up to 26 cm (10.2”) from tabletop to beam center and up to 454 kg (1000 lb) or an Eulerian cradle (for diffraction experiments from a single crystal). Variable sample to monochromator distance (from 206 cm (81”) to 236 cm (93”)) and sample to detector distances (from 61 cm (24”) to 173 cm (68”)) will allow the user to select the $Q$ range covered by the PSD. Optical benches, both inside and outside the shutter, will make customization and upgrades of the neutron optical components simpler to implement. An increased number of motorized axes as well as additional supporting software provided by a dedicated programmer in the CNBT program will make this user-friendlier instrument.
A number of general areas of investigation of biological membrane and biomimetic thin film structures are currently envisioned for the AND/R instrument. These include specular reflectometry measurements to reveal the compositional depth profile along the surface normal (with spatial resolution approaching a fraction of a nanometer) as well as non-specular scattering studies of in-plane density variations and structures. The specular reflectometry can be performed on single bilayer membrane or multilayered systems to determine the location of certain macromolecular entities of biological interest, such as cholesterol, various toxins, or transmembrane proteins. Non-specular measurements of in-plane objects typically will require multilayered samples to obtain sufficient signal.

The NCNR cold source and guide combined with optimized neutron optics and the capabilities described above are expected to make measurements using AND/R especially well suited to addressing key scientific issues on biological membranes.

NCNR staff and CNBT visitors gather at the completed AND/R instrument. Left to right: Michael Paulaitis, JHU; Kevin O’Donovon, NCNR; Don Pierce, NCNR; Huey Huang, Rice; Steven White, UCI; Anne Plant, NIST Biotech; Mathias Lösche, JHU; Jack Rush, NCNR; Tom Macintosh, Duke; Joe Dura, NCNR; Susan Krueger, NCNR; Chuck Majkrzak, NCNR.