DAVE and Other Software Developments

Scientists at the NCNR, with support from the National Science Foundation via CHRNS, have developed a new software tool for the reduction, visualization, and analysis of neutron inelastic scattering data. DAVE, short for the Data Analysis and Visualization Environment, is an integrated suite of interactive software tools with a visual interface for treating and analyzing neutron inelastic scattering data sets. Using a powerful graphical interface, users can reduce their data from one of the inelastic spectrometers, make cuts through the scattering function, and fit them with the lineshape of their choice from a library of model functions.

The goal of the DAVE software package is to allow users, whose neutron scattering experience ranges from casual to expert, to reduce, visualize, and analyze their inelastic neutron scattering data sets with a minimum of effort by using a set of visually intuitive tools. The software has been in use on many of the inelastic neutron scattering instruments since January 2002 and was released to the user community in July. The source code is available from the NCNR website to run on PC, Linux, and Mac platforms. Project and download information are available at http://www.ncnr.nist.gov/dave.

New, easy to use software for reducing and fitting neutron reflectivity data is under active development at the NCNR. The new data reduction tools employ an intuitive graphical interface developed using open source software to read and process a variety of raw data files, including specular scans, background measurements, rocking curves, polarized beam, and slit scans. Using these new tools, the user can perform a variety of data correction and manipulation tasks to produce reduced data sets of the sample reflectivity as a function of wavevector. The software supports a wide range of data formats from both the NG-7 and NG-1 reflectometers and single channel or multichannel, position-sensitive detectors.

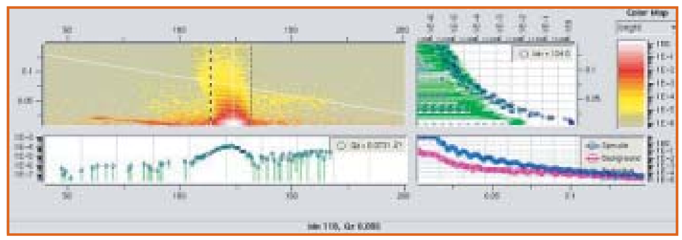

Fig. 2. Graphical interface image of neutron reflectivity data obtained using a position sensitive detector with corresponding slices of constant wavevector.

A new graphical interface has also been developed for the reflectivity-fitting program ‘mlayer’ [1]. This program allows users to model and fit scattering length density profiles to measured reflectivity data. The new interface for this program provides a wide set of graphical tools for adjusting and refining model parameters, controlling the fit, and constraining the model profile. A similar graphical interface has also been developed for the program that treats polarized neutron reflectivity data. Further information on these tools is available at the website: www.ncnr.nist.gov/programs/reflectometry/software.

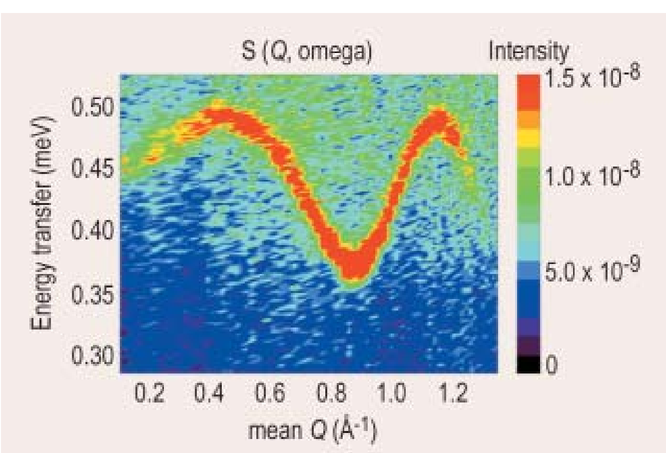

Fig. 1. An example of DAVE output: Dispersion curve of a magnetic excitation as measured using the Disk Chopper Spectrometer.

New Monochromator Drum Shields

This year the NCNR ordered two new monochromator drum shields for the new BT-7 neutron triple axis spectrometer and for the BT-4 filter analyzer instrument. Fabrication and testing of one of these drum shields has been completed and delivery of both is planned for Dec. 2002.

Monochromator drum shields are a key component in crystal spectrometers, forming a thick, moving shield that surrounds the intensely illuminated monochromator and allowing the diffracted beam to be directed at a variety of take-off angles towards the sample. The design of the new drum shields is based on a concept originally developed for the Advanced Neutron Source project at Oak Ridge National Laboratory which uses pairs of counter-opening shield wedges to allow the large diameter neutron beams to enter the drum. For the NCNR drums, this design concept was adapted for the specific dimensions of the NCNR source and to optimize the manufacturability of the shield. This double wedge design uses a precision cam track to position the shield wedges around the 20 cm beam opening as the drum is rotated to various take-off angles. The drum shield is rotated using a stepper motor driven gear system. The take-off angle range is between 0° and 120° and the drum can be built into either clockwise or counter-clockwise rotating models. The NCNR will be the first neutron laboratory to implement this double-wedge design for a monochromator shield.

Fig. 3. George Baltic (center, NCNR) confirms completion of a monochromator drum with Paul Brand (left, NCNR) and Rich Porter, president of Ingersol Contract Manufacturing Company.

Sample Environment Equipment

The suite of available sample support equipment at the NCNR continues to be upgraded and enhanced. This year, the superconducting magnet system with dilution refrigeration was upgraded from the seven Tesla coils available last year to the full design field coils that provide 11.5 Tesla. This system has demonstrated a 22 mK base temperature and full magnetic field strength.

The NCNR also received a new nine Tesla horizontal field superconducting magnet with single crystal windows using a design specifically optimized for small angle scattering experiments. This system uses a split coil design and windows in either direction to allow the magnetic field to be directed parallel or perpendicular to the neutron beam axis. Extensive heat shielding extends operation of the magnet to the higher sample temperatures needed for biology or polymer physics experiments without significantly altering liquid helium consumption.

Other new equipment made available this year includes a pulse tube closed cycle refrigerator (CCR) with an operating temperature range of 3 K to 325 K, two low temperature CCRs (10 K to 325 K), one high temperature CCR (15 K to 800 K), one 50 mm helium cryostat (1.5 K to 300 K) and fifteen additional temperature controllers.

Facility Improvements

Taking advantage of the opportunity provided by an extended interruption in routine operations, the NCNR staff completed several improvements to the facility during the outage early this year. The helium gas blanketing system, which provides a continuous flow of helium gas to the first 1.5 m of neutron guide closest to the cold source, was replaced with a new gas control system. Sensors and controllers on the guide vacuum systems were replaced and upgraded during the cold source installation. A computerized supervisory and control system for the facility was expanded to include monitoring of the guide vacuum pumping system.

Several improvements were made in C100, the location of the thermal neutron instruments. These include the installation of wiring and breaker panels that are part of a new power distribution system for the thermal instruments. The new system provides each neutron station with independent panels and outlet locations at the floor level adjacent to the experimental work area. A new catwalk system was also designed for accessing the face of the biological shield above the thermal instruments. This will be a significant safety and performance improvement for maintenance activities in this area. A prototype for a perimeter shield was also accepted this year. The perimeter shields surround the thermal neutron spectrometers and separate the operating area of the spectrometers from other work areas on the floor.

In the Guide Hall, the concrete floor was repainted. The original surface was badly worn and needed replacement. A three-color design was adopted to help differentiate work areas, walkways, and fire protection equipment.

References

[1] J.F. Ankner and C.F. Majkrzak, SPIE **178**, 260 (1992).