Fig. 2. Display prepared for the 2003 American Crystallographic Society meeting

Fig. 3. Left to right: Jim Viccaro (Executive Director, Consortium for Advanced Radiation Sources; Principal Investigator, ChemMatCARS, APS sector 15; and Chair, APS Partner User Council), Pedro Montano (Program Manager for X-ray and Neutron User Facilities, DOE-BES), and Alec Sandy (XFD) meet at the APS exhibit at the fall 2003 Materials Research Society meeting.

dees stopped at the APS booth to pick up materials, discuss potential research opportunities, and learn how to use the on-line proposal submission system. An equally successful venture was an exhibit at the December 2003 Materials Research Society meeting in Boston, which had an attendance close to 5000. Figure 3 is a photo taken at the APS exhibit during that meeting. ❍

NEWS FROM APS USER GROUPS

The Inelastic X-ray Scattering Collaborative Development Team (IXS-CDT) and the Nanoprobe-CDT at the ANL Center for Nanoscale Materials (CNM) are the 22nd and 23rd research groups, respectively, to sign Memoranda of Understanding (MOUs) for construction of x-ray beamlines at the APS. (Collaborative development teams represent a new kind of partner-user arrangement at the APS. They are similar to the more traditional collaborative access team during the construction and commissioning phases but becomes an APS facility beamline during operations, open to competitive access by both general and partner users.)

Fig. 4. Pens at the ready, ANL Associate Laboratory Director and APS Director Murray Gibson (left); John Hill (BNL), Executive Director of IXS-CDT; ANL Deputy Laboratory Director Donald Joyce; and Miles Klein (U. of Illinois at Urbana-Champaign), IXS-CDT Executive Board Chairman, prepare to sign the IXS-CDT Memorandum of Understanding at a ceremony held at the APS.

IXS-CDT

With strokes from four ceremonial pens at a September 15, 2003, MOU signing ceremony (Fig. 4), the IXS-CDT became the 22nd research group to sign up for construction of x-ray beamlines at the APS. APS staff will construct the IXS-CDT beamline at sector 30 on the APS experiment hall floor. John Hill (Brookhaven National Laboratory) is the Executive Director of IXS-CDT; Ercan Alp (ANL/XFD) is the Managing Director.

The IXS sector intends to be the best in the world for inelastic x-ray scattering, a critical synchrotron x-ray application that takes full advantage of the brilliance from third-generation synchrotrons such as the APS. The IXS-CDT will have two specialized spectrometers: HERIX, a high-resolution inelastic x-ray scattering instrument for studies of lattice vibrations, and MERIX, a medium-resolution spectrometer for electronic structure measurements.

Members of IXS-CDT come both from the existing inelastic x-ray scattering community and from the broader scientific community that could benefit from access to such an instrument. Member institutions are the Massachusetts Institute of Technology; Northeastern University; Princeton University; the State University of New York, Stony Brook; Stanford University; the Universities of Akron (Ohio), California (San Diego), Illinois at Chicago and Urbana-Champaign, Tennessee, and Pennsylvania; and Western Michigan University; the Argonne, Brookhaven, and Oak Ridge national laboratories; the Carnegie Institute of Washington; the Albert Einstein College of Medicine; and Lucent Bell Laboratories.

Planners believe that the strength of IXS-CDT lies in a broad scientific program ranging from condensed matter physics to polymer science and biology, and the resources that members bring to the consortium. Understanding the dynamics of a material's molecular system is crucial from a number of perspectives. For researchers interested in hard condensed matter, a given system is completely described by the relaxed electronic state of molecules (called the "ground state") and the excitations from that ground state. From a soft condensed matter perspective, the propagation of sound waves and other density fluctuations determine the response of the system to time-varying probes—a key aspect of the properties of a material.

< Artist's rendering of the Center for Nanoscale Materials at Argonne National Laboratory.

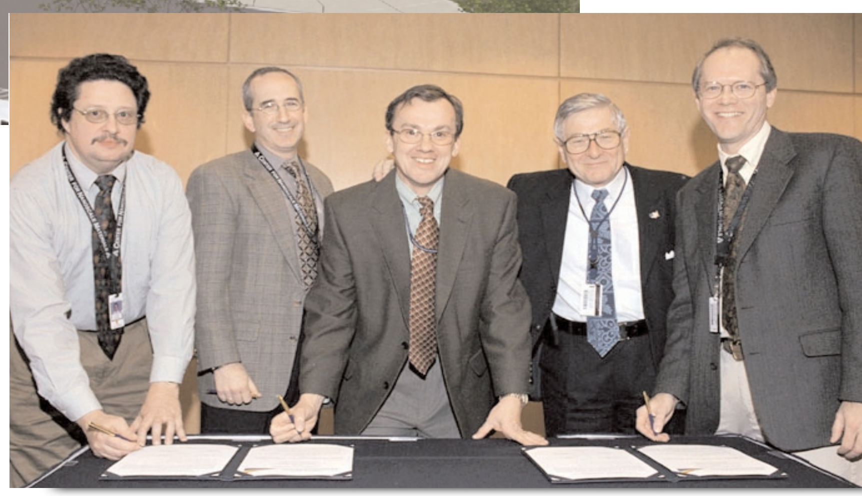

Fig. 5. Construction of the Nanoprobe beamline officially begins with MOU signatures from (left to right): Derrick Mancini (CNM Project Manager), Eric Isaacs (CNM Director), Murray Gibson (ANL Associate Laboratory Director for the APS), Hermann A. Grunder (ANL Director), and G. Brian Stephenson (Director, CNM Nanoprobe Beamline).

Nanoprobe-CDT

On December 4, 2003, the MOU between the APS and the Center for Nanoscale Materials CDT was signed by principals from ANL, APS, and CNM (Fig. 5). The MOU allocated APS sector 26 to the CNM and authorized the CNM to begin construction and commissioning of the hard-x-ray Nanoprobe beamline.

The Nanoprobe beamline will be the centerpiece of the x-ray characterization facilities at the CNM, one of five Nanoscale Science Research Centers being constructed at the Department of Energy's national laboratories. The CNM is a $72 M federal/State-of-Illinois partnership for designing, synthesizing, fabricating, and characterizing materials at the nanoscale. The CNM user facility will provide the scientific community with a broad complement of tools, including the Nanoprobe and other advanced nanocharacterization, nanolithography, and synthesis tools. CNM users will be equipped to explore problems in nanophotonics, nanomagnetism, bioinorganic interfaces, nanocarbon, and complex oxides.

The Nanoprobe, which is being constructed by the CNM organization within ANL, is the CNM's premier nanocharacterization tool, designed to afford capabilities for fluorescence, diffraction, and transmission imaging at a spatial resolution of 30 nm or better. Funding for the Nanoprobe beamline is provided by DOE's Office of Basic Energy Sciences as part of the CNM equipment budget. The Nanoprobe is expected to advance the state of the art in nanoscience by providing the highest-spatial-resolution hard x-ray beamline in the world. With advanced zone plate optics and an optimized beamline design, the performance goal is to provide a spatial resolution of 30 nm, a spectral range of 3 to 30 keV, and a working distance between the nanofocusing optics and the sample in a range of 10 to 30 mm. This unique instrument will not only be key to the specific research thrusts of the CNM but will be of very general utility to the broader nanoscience community.

The design and features of the Nanoprobe were developed with input from a broad user community, which met at several workshops. These included the workshop on “X-rays and Nanoscience” held in 2000; the “Workshop on Nanoscale Science using Synchrotron Techniques” held in 2001 concurrently with the APS Users Meeting; a separate workshop for the CNM in 2001; and a fourth workshop on “Institutes and Facilities for Nanoscience,” held during the 2003 APS Users Meeting. All four workshops were well attended, attracting hundreds of potential users who provided valuable feedback.

The BioCARS BSL-2/BSL-3 Facility: A Resource for Solving Virus & Toxin Structures

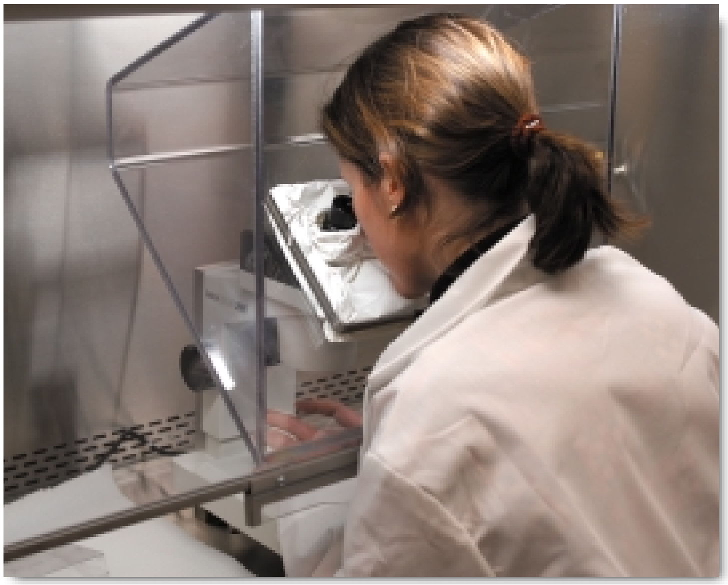

Fig. 6. BioCARS biosafety cabinet in use.

The Biology Consortium for X-ray Research (BioCARS, APS sector 14) is a national user facility that fosters frontier research in the field of macromolecular crystallography. BioCARS provides state-of-the art facilities and scientific and technical support for structure determination of macromolecules by standard x-ray diffraction techniques (such as the multiple-wavelength anomalous diffraction technique). But the facility is also designed for two special tasks that set it apart from other centers for macromolecular crystallography at the APS and nationwide. The BioCARS beamline 14-ID can serve as both a monochromatic and polychromatic x-ray source. The polychromatic capability is essential for conducting time-resolved x-ray diffraction experiments that utilize the Laue technique. These experiments result in molecular movies depicting biologically important macromolecules as they perform their function. The other special feature of the BioCARS facility is that, as the result of planned substantial HVAC upgrades, all three experimental stations will be embedded in a Biosafety Level (BSL) 3 containment, unique at the APS and nationwide. This permits safe research with biohazardous materials classified as Biosafety Level 2 or 3 agents, such as human, animal, or plant viruses and toxins.

Agents classified as BSL-2 involve a broad range of indigenous moderate-risk agents that are present in the community and associated with human diseases of varying severity. Immunization or treatment for these agents is available. Examples include the measles and hepatitis B viruses, and *Salmonella.* Agents classified as BSL-3 are indigenous or exotic agents that may cause serious and potentially lethal human diseases as a result of exposure by the inhalation route. Examples of BSL-3 agents include *M. tuberculosis*, St. Louis encephalitis virus, and *Coxiella burnetii*. The guidelines for BSL-2 and BSL-3 facilities, described in the “Biosafety in Microbiological and Biomedical Laboratories” CDC/NIH publication (Fourth Edition, May 1999), require special safety equipment as well as a special facility design for the handling of BSL-2 and BSL-3 materials. Manipulation of all BSL-3 agents is done in a Class II biosafety cabinet (Fig. 6) that serves as the primary barrier. The facility is physically separated from access corridors and must be maintained under negative pressure with respect to the APS experiment hall while BSL-2 and BSL-3 experiments are being conducted. The air flows into the laboratory and is exhausted via a HEPA filter out of the APS building. Mandatory special operating procedures for BioCARS users and staff are being developed. They describe in detail the rules for conducting BSL-2 and BSL-3 experiments and responding to incidents and emergencies, as well as the safe disposal of any waste generated during such experiments.

The primary scientific and practical expertise for the work with BSL-2 and BSL-3 agents resides with BioCARS users. Many virus crystallographers nationwide already use the BioCARS facility for their research projects. In this expanding field of national importance, BioCARS is in a position to play an important role as the only synchrotron-based x-ray diffraction laboratory that can be used for the safe study of these samples. The facility is to be fully operational in 2004 *(Contact K. Brister, brister@cars.uchicago.edu.)*

Bio-CAT Helps Facilitate Fiber Diffraction Network

A number of Biophysics Collaborative Access Team (Bio-CAT) researchers, including Bio-CAT director Tom Irving, are helping to lead the newly formed, National Science Foundation-funded project “FiberNet,” which coordinates the development of biological fiber diffraction methods, focusing particularly on computational methods. Activities will include the development and integration of software for biological fiber diffraction and exchange of information about fiber-diffraction methods through retreats, workshops, and a public Web site.

Perhaps the best-known achievement of fiber diffraction was the determination, 50 years ago, of the DNA structure by Crick and Watson, using the fiber diffraction data of Rosalind Franklin. Fiber diffraction continues to be an active and important area of structural biology, focusing on large biological assemblies, such as viruses and muscle fibers. The use of fiber diffraction in biological structure determination has been reviewed by Chandrasekaran and Stubbs (2001). Many biopolymers are long helical structures and have a natural tendency to form fibers. This tendency severely impedes the growth of single crystals. Even if crystals can be grown, the molecular interactions in the crystals rarely correspond to the biologically significant interactions in the fibers. Conventional crystallography is, therefore, often not applicable to these systems. Fiber diffraction is a powerful technique for determining the structural details of such polymers.

In the new network, software applications particularly concerned with structure determination and model refinement will be adapted to various platforms, integrated with the suite of programs available through the British Collaborative Computational Project for Fibre Diffraction (CCP13), and made available to the scientific community. New software will be developed where existing software is inadequate. The network software will be complementary to CCP13 software; together, they will eventually cover all aspects of biological fiber diffraction.

The network will also integrate U.S. fiber-diffraction groups with each other and with the world fiber-diffraction community, particularly with CCP13. This will be done through workshops organized by the core participants, including workshops at the Bio-CAT facility at the APS, and through partial sponsorship of sessions organized by the Fiber Diffraction Special Interest Group of the American Crystallographic Association (ACA SIG).

Membership in the network and participation in its activities will be open to all who are interested in the development of fiber diffraction. Through the ACA SIG, the user group of Bio-CAT, CCP13, and the network's own Web site, the group expects to reach virtually all interested parties. Network activities will directly impact the fiber diffraction community, particularly the biological fiber diffraction community, in the U.S. and internationally. They will also benefit the small-angle-scattering community and other groups using diffraction methods to study partially ordered molecular structures. Stay tuned for the release of the Web site address. More information on Bio-CAT can be found at http://www.bio.aps.anl.gov.

See: R. Chandrasekaran and G. Stubbs, "Fibre diffraction," *International Tables for Crystallography, Vol. F: Crystallography of Biological Macromolecules*, M.G. Rossman and E. Arnold, eds., 444-450 (Kluwer Academic Publishers, The Netherlands, 2001). *(Contact G. Stubbs (FiberNet Director), stubbs@vanderbilt.edu, or T. Irving, irving@iit.edu.)*

Nadia Leyarovska (left, the University of Georgia and SER-CAT) and Zhongmin Jin (the University of Georgia and SER-CAT) logging in crystal shipment for the Mail-In Crystallography Program.

Beamline Time Sharing at SER-CAT: Mail-in Crystallography & Remote User Participation

A major long-term goal for the Southeast Regional CAT (SER-CAT) is realizing the concept of providing its members with time-sharing of beam time. The purpose of this goal is to maximize the use of members' yearly allocated beam time (proportional to the shares that a member owns), increase the flexibility and frequency of a member's access to SER-CAT's beamlines, and reduce the travel expenses needed for data collection. Toward these ends, SER-CAT has initiated a mail-in crystallography program for members in order to work out the logistics of administering such a program. In the 2003-2 APS run (January-March 2003), a total of 24 h of beam time in five slots were allocated to the mail-in program, and SER-CAT staff collected data for nine research groups from seven institutions.

There is a disadvantage to mail-in crystallography because users cannot actively participate in the data collection. However, SER-CAT personnel are planning to test the feasibility of user remote participation through fast internet communication with resident scientists at SER-CAT's beamline. Once this program is implemented, a user sitting 10 feet or 1,200 miles from the experimental hutch can conduct research via actively participating in data collection and interacting with SER-CAT on-site personnel. This is one of several areas of research SER-CAT is pursuing to provide its members with the most effective use of available beam time for synchrotron macromolecular crystallography. *(Contact J. Chrzas, chrzas@anl.gov)*

UNI-CAT 34-ID BEAMLINE UP & RUNNING

The University-National Laboratory-Industry CAT has declared the sector 34 undulator beamline operational.

The 34-ID insertion device beamline is a dual-purpose beamline that supports coherent x-ray diffraction and x-ray microprobe techniques. This beamline is designed and constructed in a tandem configuration (not to be confused with the canted undulator configuration) based on a single APS undulator A and uses a horizontally deflecting mirror to split the beam into pink- and white-beam branches. The pink beam supplies a coherent x-ray diffraction (CXD) experiment with a general-purpose diffractometer. A diamond-crystal monochromator may be inserted to permit studies with monochromatic radiation. The white-beam branch provides a microfocus diffraction (MFD) experiment and includes an optional monochromator in the third optics enclosure. Both experiments are brilliance limited and can accept only a fraction of the divergence from the source. For this reason, the beam-splitting mirror, which divides the undulator beam, does not compromise the flux in either experiment.

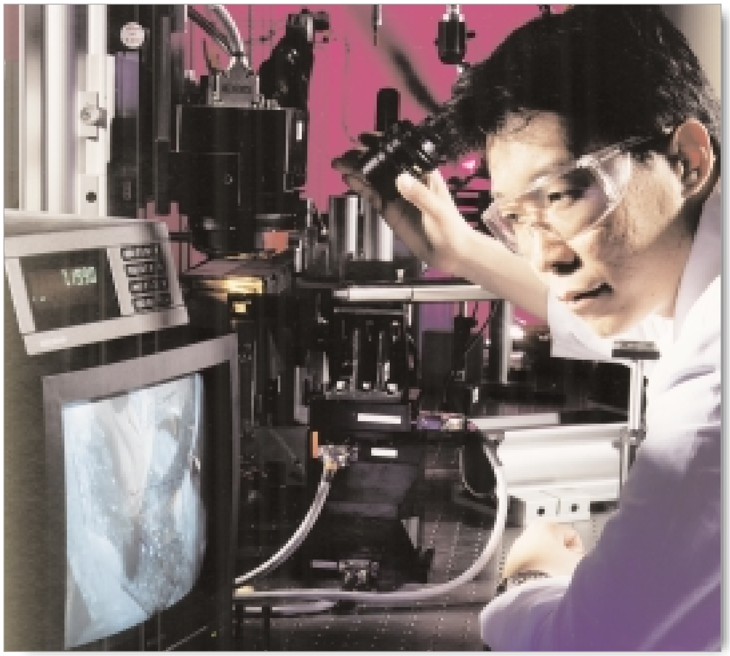

Fig. 7. Wenjun Liu (University of Illinois) aligns a sample and prepares for a differential aperture scan in the 34-ID-E microbeam station.

The coherent x-ray diffraction experiment station, 34-ID-C, contains a specialized goniometer, which permits both vertical and horizontal scattering geometries and accommodates an ultrahigh-vacuum chamber to permit studies at clean surfaces. A Kirkpatrick-Baez (K-B) focusing mirror system provides micron-scale beams that preserve the beam coherence.

The microbeam station at 34-ID-E, as shown in Fig. 7, produces x-ray beams that are routinely 0.4 µm x 0. 4 µm or better for use in diffraction or fluorescence techniques using K-B focusing mirrors. The specially designed micromonochromator allows the selection of either white or monochromatic conditions with a fixed focal spot on the sample. Diffraction techniques with this small spatial resolution permit careful examination of the stress-strain state of materials. Newly developed differential aperture microscopy techniques permit the microprobe to reveal diffraction information in order to determine the structure and/or orientation of small volumes within a solid sample and to provide spatial resolution of better than 1 µm in all three dimensions.

The development of the CXD instrument was funded by the Major Research Instrumentation program of the National Science Foundation, while the microbeam experimental capabilities were sponsored by the DOE Office of Basic Energy Sciences. In addition, through the Illinois Board of Higher Education, the State of Illinois has provided considerable support for construction and continuing operations. *(Contact P. Zschack, zschack@anl.gov.)* ❍

USER SUPPORT

NEW USER-SUPPORT PERSONNEL

The **Beamline Technical Support Group (BTS)** works from the premise that each sector need not require its own complement of specialists. The BTS Group applies technical and administrative expertise to user instrument and facility engineering and design, the spare-equipment pool, and a dedicated material handler, and facilitates user access to a variety of APS resources, such as AutoCAD.

The **User Technical Interface** is the person empowered as the primary contact point between users and the three APS divisions in matters related to beamline technical information. This person assures the quality and availability of the huge storehouse of documentation needed by APS operations staff, as well as the users, for successful beamline operations in accordance with APS policies and procedures.

User Policy and Planning is the responsibility of the individual who works in close cooperation with users to establish the policies and procedures that govern researchers' access to the APS and their workplace activities while they're here. This person also coordinates user support activities that require interaction between APS organizations, including records and material handling; interdivisional beamline construction schedules; exchanges between users and APS technical staff regarding the installation of beamline shielding, utilities, personnel safety systems, front ends, and insertion devices; and reviews of beamline design and management and safety plans.

As the first APS ombudsman, this person is also a conduit to APS management for other issues raised by users.