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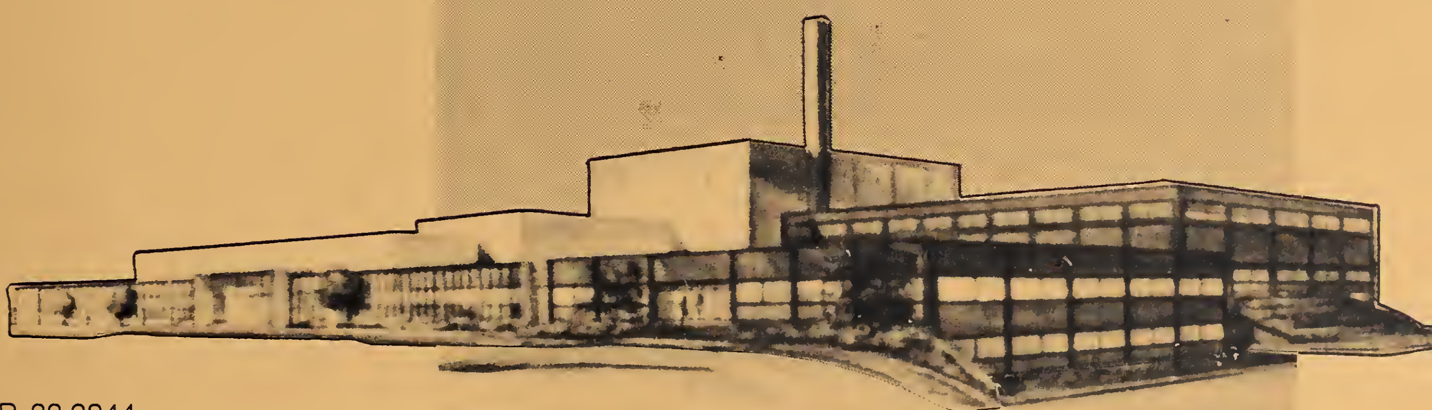
Institute for Materials Science and Engineering

REACTOR RADIATION



NAS-NRC
Assessment Panel
December 6–7, 1988

NISTIR 88-3844
U.S. Department of Commerce
National Institute of Standards
and Technology

Technical Activities 1988

Artist's Rendering of the NBS Research Reactor with the adjoining neutron guide hall and office/lab wing that will constitute the Cold Neutron Research Facility.

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REACTOR RADIATION

R.S. Carter, Chief
T.M. Raby, Deputy

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ABSTRACT

This report summarizes all those programs which depend on the NBS reactor. It covers the period from October 1, 1987 through September 30, 1988. The programs include the application of neutron methods to the characterization of materials, neutron standards, trace analysis by neutron activation analysis, neutron depth profiling, nondestructive evaluation, and the production of radioisotopes.

Key words: Activation analysis; crystal structure; diffraction; isotopes; molecular dynamics; neutron; neutron radiography; nondestructive evaluation; nuclear reactor; radiation.

DISCLAIMER

Certain trade names and company products are identified in order to adequately specify the experimental procedure. In no case does such indentification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the products are necessarily the best available for the purpose.

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OVERVIEW

REACTOR RADIATION DIVISION (460)

Robert S. Carter, Chief
Tawfik M. Raby, Deputy Chief
S. E. Tassey, Secretary

The dual responsibilities of the Reactor Radiation Division include the operation and maintenance of the National Institute of Standards and Technology* reactor (NBSR), and the conduct of a program in materials research and characterization which also provides the core expertise to establish the NBSR (augmented by a Cold Neutron Research Facility, CNRF, currently under construction) as a national center for the application of reactor radiation to a variety of problems of national concern. The major areas of activity are:

Reactor Operation and Irradiation Services
Materials Characterization
Nondestructive Evaluation
Trace Analysis
Radiation Standards and Measurement

The Reactor Radiation Division (RRD), in collaboration with other scientists within the Institute for Materials Science and Engineering (IMSE), other NBS Centers, and many outside organizations uses neutron scattering methods to determine the properties and behavior of materials at the submicroscopic level. These methods are used to study a wide variety of problems in such areas as hydrogen in metals, microstructure of ceramics , metals and polymers, microscopic properties of advanced crystalline and amorphous magnetic materials and superconductors; and molecular species, interactions and pore structures in catalysts and microporous materials. NIST is in an excellent position to carry out such a multidisciplinary program because of its strong materials programs located in IMSE and other centers and its 25 state-of-the-art reactor facilities that are not available in private-sector laboratories. A major expansion of these facilities are now underway that will add a 20,000 $ft.^2$ cold neutron guide hall and 15 instruments, most of which are currently unavailable anywhere in the United States.

Major Activities:

The major research activities of the Reactor Radiation Division involve developing state-of-the-art neutron diffraction, inelastic scattering and radiographic methods and associated experimental facilities, and fostering their application by NIST divisions and offices and other U.S. industrial, university and government groups to meet critical research needs in physics, chemistry, materials science, and biology. The scientific core group maintains essential research capabilities in condensed-matter science and engages in cooperative research with some 220 scientists from NIST and

*In August, 1988, the name of the National Bureau of Standards was changed to the National Institute of Standards and Technology.

outside groups in areas of new high technology magnetic and amorphous materials, modern electronic and structural ceramics, high-temperature superconductors, chemical catalysts, advanced metals and alloys, and thin films being developed for new products and technological applications.

In the area of nondestructive evaluation (NDE), RRD uses neutron radiography and both large and small-angle neutron diffraction to examine objects for defects or hidden components that must be examined nondestructively. The major effort is in the development of new or improved neutron NDE methods. Methods are being developed for such diverse applications as the use of autoradiography to study rare paintings and the use of neutron scattering to investigate voids, strains, and other defects causing failure in structural materials.

Neutron activation analysis is a very sensitive technique for measuring trace elements at very low concentrations. RRD provides the sample irradiations, but the program and sample analysis is carried out by the Center for Analytical Chemistry (CAC). Activation techniques are used extensively for characterizing Standard Reference Materials (SRM) and a variety of other measurements such as the determination of Iodine-129 concentrations and environmental studies. A large number of outside organizations also use these techniques for measuring trace elements or pollutants in foods and drugs, environmental samples, criminal artifacts, etc. This is one of the largest neutron activation analysis programs in the country with thousands of samples irradiated each year. Although the primary effort in this activity is centered around neutron activation analysis, other neutron analytical methods are also being developed. A facility has been built to analyze for trace elements by measuring the prompt gamma ray spectrum induced by neutron capture in the sample, and a facility has been developed (depth profiling) to measure concentrations of light elements (e.g., B, Li) as a function of depth with ~ 100 A resolution, which is the best in the United States. New, greatly advanced, prompt gamma ray and neutron depth profiling instruments are being developed to take advantage of the new guide hall facility presently under construction.

A program in radiation standards and measurements is carried out by the Center for Radiation Research (CRR). Through the use of double fission chambers and a series of accurately calibrated fission foils, they provide the basis for reactor neutron flux and power density measurements needed in the U.S. fast-flux development program. The calibration and intercomparison of the series of fission foils makes use of standard reference neutron fields established in the thermal column of the NBSR. CRR also maintains well characterized, filtered neutron beams in the reactor of 2 keV, 25 keV, and 144 keV energy for the calibration and development of personnel neutron dosimeters.

A number of other groups both within and outside NIST utilize the long-term irradiation facilities at the NBSR for activities ranging from γ-ray and x-ray physics and standards to application of isotopes in medical diagnosis.

Highlights of FY 88 Accomplishments:

The cold neutron source was installed in August, 1987. A series of start up tests were performed to determine the release during warm up of the radiolytic products (D_2 and O_2) as a function dose. The results confirmed the expectation that the ice could be maintained frozen for an indefinitely long period of time without build up of excessive levels of radiolytic gases. In fact, the frequency of the replacement of the moderating ice is determined by the amount of tritium that builds up from neutron capture in the deuterium. In order to maintain the tritium concentration below a prudent level (a level comparable to that in the main D_2O reactor coolant), the ice needs to be changed only every third reactor cycle or about every four months. The start up tests also showed that the cold source performance could be improved by the addition of some H_2O. The optimum concentration was determined to be 7 1/2%. The gain in intensity for long wavelength neutrons was found to be about a factor of five for the cold source filled with the ice moderator at low temperature (~35k) versus the empty ice chamber.

Construction of the new cold neutron guide hall and support facilities began in November, 1987, and is over 80% complete. Beneficial occupancy is scheduled for January, 1989; current progress may allow earlier occupancy. The construction has gone well, with a minimum of change orders, reflecting both a good design package and excellent management by the Plant Division. The neutron guide complex has been fully designed, and construction is underway with the first delivery planned for March, 1989. Detailed design of four instruments is complete, with fabrication begun on all four (SANS, depth profiling, prompt gamma, and neutron physics). A diverse program of advanced instrumentation R & D is well underway, and several tests of new concepts have been successfully completed. Five other instruments are at various stages of design and construction (advanced time-of-flight, triple-axis spectrometer, reflectometer, back scattering). An extensive set of computer simulation codes for instrument design are now in place giving us an unrivaled advanced R & D capability.

Accomplishments in our neutron scattering research programs during the past year include new structure studies of high T_c superconductors (with Johns Hopkins) which show that atomic disorder on "plane" sites in 1, 2, 3, superconductors is much more detrimental to superconductivity than "chain" site disorder, thus strongly suggesting a more critical role of the planes in the superconducting interaction. Further work with AT&T has defined three crystallographic building blocks which can be arranged to reproduce the structure of all known high T_c superconductors - thus providing a predictive tool for synthesis of new compounds. In magnetism studies we have, e.g. (with Bellcore) determined the details of antiferromagnetic ordering in high T_c superconductors, including its temperature dependence and determined for the first time the pair-wise exchange interaction in dilute magnetic semiconductors (with Notre Dame). In our research on catalysts-pillared clays (with Michigan State and Schlumberger-Doll) and zeolites (with ICI and the University of California) - we have obtained new information on the orientation of pillaring ions along with spectroscopic determination of the torsional potentials of intercalated tetramethyl ions. These results provide the first experimental information to test current models of the interlayer template potential of a clay. Detailed information of the rotational potential of H_2 adsorbed in zeolites has also been obtained by time-of-flight and energy-loss spectroscopy. In our research efforts on hydrogen in metals we have confirmed by vibrational spectroscopy (with KFA, Jülich), the existence of a complex bimodal distribution of site energies for H dissolved at low levels (≥0.1%) in a metallic glass ($Pd_{.85}Si_{.15}$). In the area of submicron materials structure we have recently extended our research to develop neutron reflection and grazing angle diffraction as powerful probes of surface and infacial structure. As an example, we have carried out (with IBM) a dramatically successful first study of lamellar formation and surface ordering in diblock copolymers and have demonstrated the ability to measure reflectivities as low as 10^{-6}. In the area of SANS, new theoretical methods developed to analyze multiple scattering by large microstructural features have been applied to characterize the porosity at various stages of densification of sol-gel synthesized silica materials. A successful description of the SANS from the highly regular pore structure in controlled pore glasses has also been achieved using our recent theoretical results in the modeling of bicontinuous structures.

Finally our crystallographic efforts have included research on the crystal chemistry of high T_c superconductors and related ceramics and studies of ring ellipticity parameters affecting the molecular exchange in zeolite-rho catalysts (with Dupont) and on the structure of highly catalytic phases of partially dehydrated aluminum hydroxide (with Alfred University). In addition our crystal data activity has produced (with Sandia) a new Electron Diffraction database and started the process to obtain a patent on a new Matrix approach to symmetry which promises to greatly enhance automated diffractometry in the laboratory.

Reactor Utilization:

As is indicated earlier, RRD has a dual function. It conducts research programs in the areas of materials research and NDE and serves as a focal point of neutron scattering expertise for many other programs both within and outside of NIST. The second function includes not only the operation of the reactor, but also the provision of sample irradiation services for a large number of users.

An important part of the overall Reactor Division contribution to the NIST mission and to the scientific and technical community is in fostering the utilization of the reactor by other NIST groups and outside organizations. Interactions with other scientists and organizations take the form of both collaborative efforts and independent programs which rely on utilization of the reactor and facilities provided by the NBSR staff. The extent of such interactions for FY 88 are indicated in the tables below. The number of personnel shown in Tables 1 and 2 include many short-term collaborators as well as permanent other agency and university guest workers. These numbers are constantly changing and so may not be exact.

Collaborative interactions are those in which workers from outside the RRD collaborate scientifically with RRD scientists on problems of mutual interest. These interactions are summarized in Table 1.

Many of the other agency, university, and industrial collaborators have worked with us regularly for many years. Others come from all over the world to spend a few days, weeks, or months to carry out specific experiments using the facilities available at the NBSR. Collaborative programs include measurements on new magnetic materials and superconductors, fast-ion conductors, polymers, thin films, catalytic materials, hydrogen embrittlement, voids and precipitates in alloys, and ceramics, etc.

Table 1. Collaborative Interactions

	No. of Personnel FY 88
RRD Permanent Scientists	19
Non-RRD Participants	
Other NBS	31
Other Agency	35
University	76
Industrial	42
International	39
Total Non-RRD	223

Independent programs are those programs carried out independently of the Reactor Radiation Division scientific staff by other NBS Divisions and outside organizations. Table 2 summarizes these interactions.

Table 2. Independent Programs

	No. of Personnel FY 87
Other NBS	32
Other Agencies	33
Universities	40
Industrial	18
International	5
Total	128

These tables demonstrate the extensive utilization of the NBS reactor by scientists and engineers from outside the Division. They come from 14 NBS Divisions and offices, 17 other Federal organizations, 45 U.S. universities, 22 U.S. industrial laboratories, and 23 foreign laboratories.

Organization of Technical Activities:

The technical activities of the Division are organized into major tasks. These are summarized below and described in more detail in the "Description of Technical Activities" section. Because the reactor serves not only the Reactor Radiation Division and IMSE, but many other NBS Centers and outside organizations, a description of the major outside activities (Independent Programs) will also be included.

REACTOR OPERATIONS AND SERVICES

This task operates and maintains the NBSR, handles all licensing interactions, reactor security, and provides sample irradiation services to a large variety of users. Services range from pneumatic tube irradiations for neutron activation analysis to the production of radioisotopes for medical research.

NEUTRON SCATTERING CHARACTERIZATION OF MATERIALS FOR ADVANCED TECHNOLOGIES

This task develops and applies neutron scattering methods and related theoretical analysis for research on the fundamental properties of materials which affect their use in technological applications. Current areas of emphasis include new magnetic and superconducting materials, hydrogen in metals, catalytic materials, layered materials and thin films. A variety of inelastic neutron scattering methods are utilized to probe the key submicroscopic properties of these new materials. Task scientists also utilize the special role of neutrons in the structural analysis and nondestructive testing of materials, including concentrated efforts in neutron diffraction, small angle scattering, profile refinement, and state-of-the-art computer methods for: (1) precise structure and microstructure analysis for effective use of materials (e.g., in electronics, advanced transportation systems, and chemical catalysis), (2) development and transfer of an evaluated materials structure database, (3) nondestructive reference methods for texture, and strains affecting materials product processing and performance. The members of this task are also responsible for establishing and maintaining a national center of excellence for neutron scattering, including a computer-controlled network of nine spectrometers at the reactor. They further carry out the maintenance, operation, and improvement of the D_2O ice cold neutron source.

COLD NEUTRON RESEARCH FACILITY

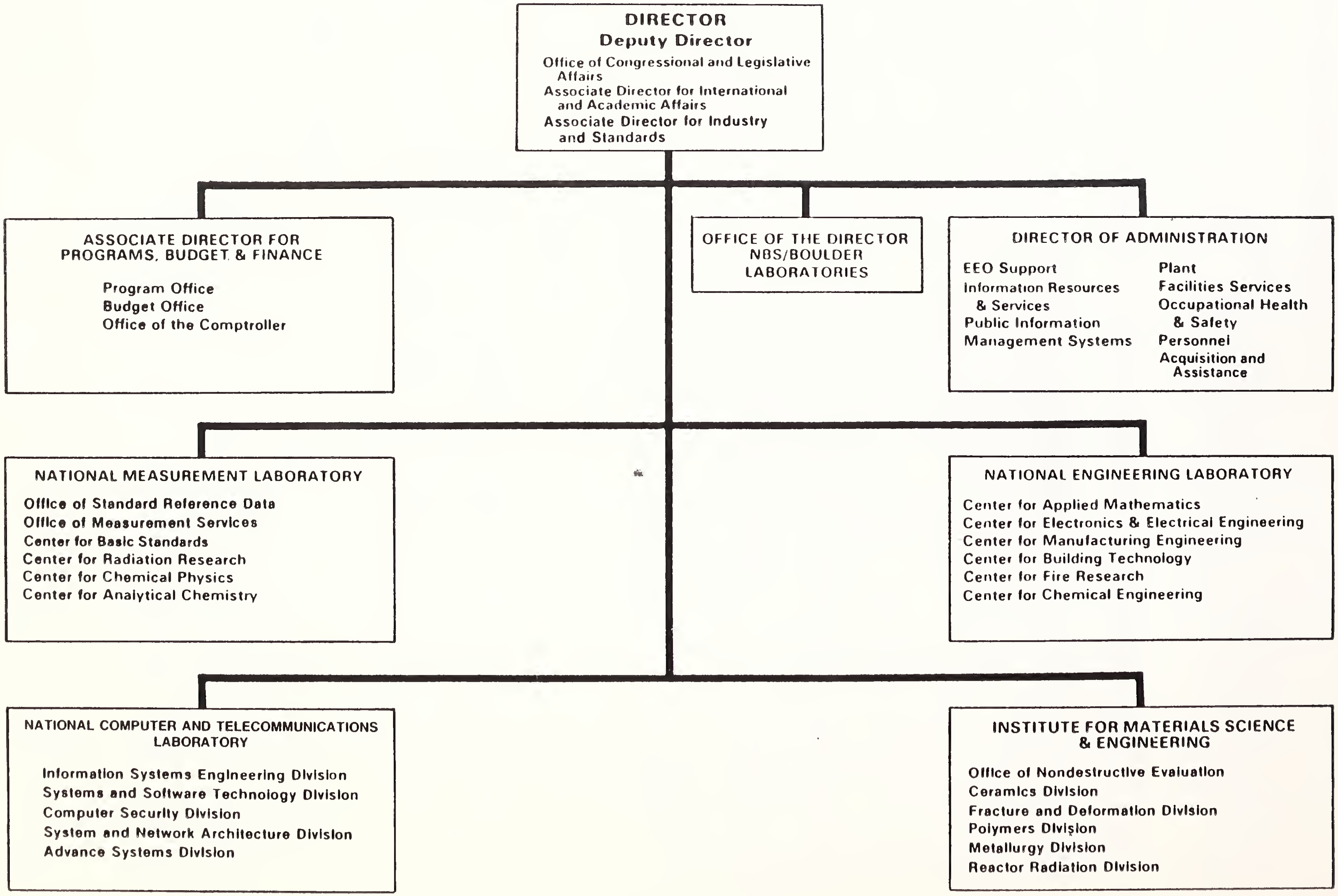
The goal of this program is to develop, install and operate a national facility for cold neutron research at the NBS reactor. This includes the design and construction of an extensive neutron guide tube network and a neutron guide hall with fifteen major experimental stations for research in condensed matter and material science, biology, and fundamental physics and metrology.

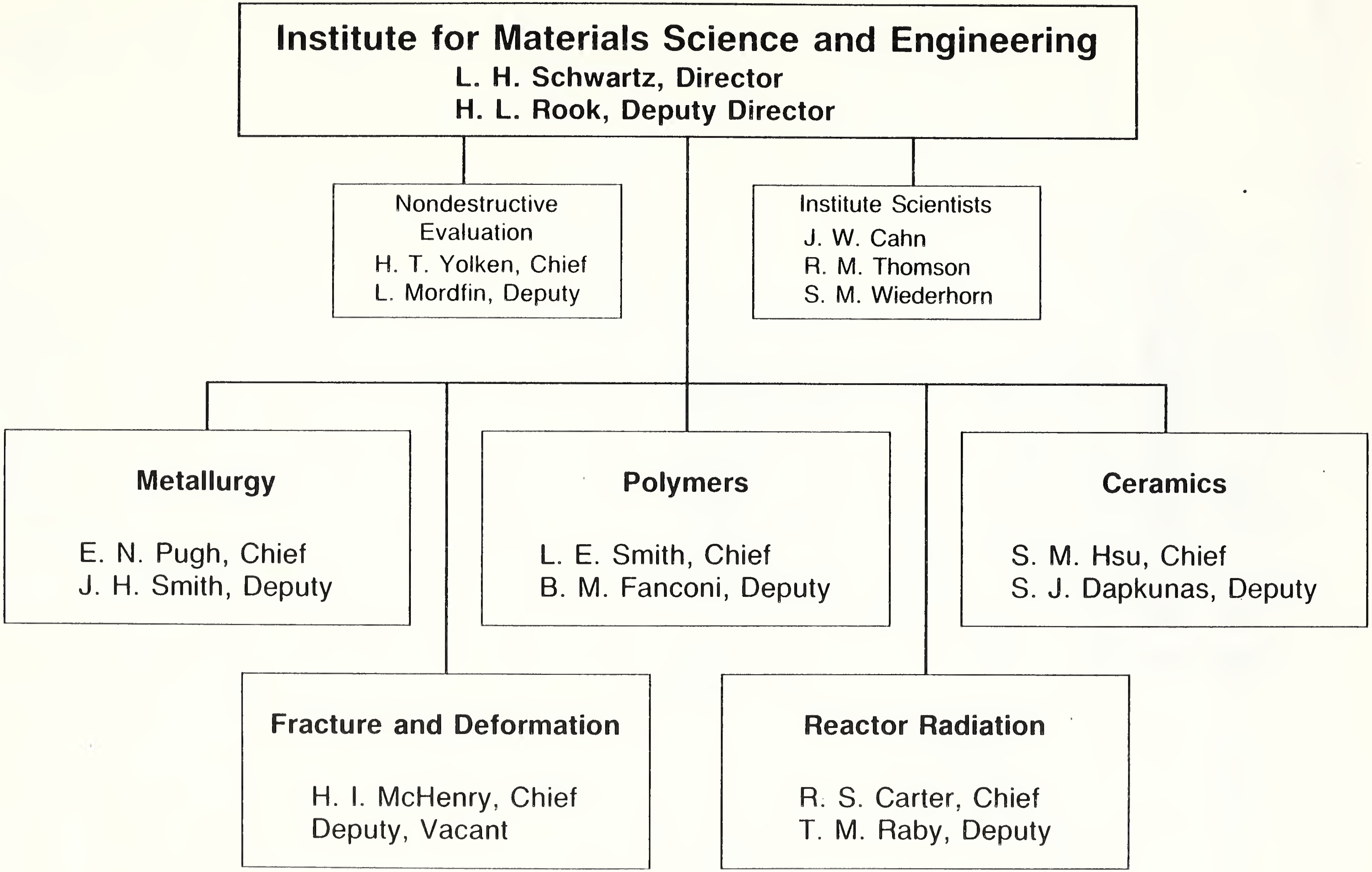
INDEPENDENT PROGRAMS

Although a great deal of research by non-Division scientists is carried out in collaboration with Division scientists, there are many research projects that utilize the reactor and its services, but which are designed and carried out without any scientific collaboration with the Reactor Radiation Division. These independent programs typically include, trace analysis, depth profiling, radiation standards, neutron dosimetry, environmental studies, and medical research.

ORGANIZATION CHARTS AND RESEARCH STAFF

U.S. DEPARTMENT OF COMMERCE
National Institute of Standards and Technology





Institute for Materials Science and Engineering
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H. T. Yolken, Chief
L. Mordfin, Deputy
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R. M. Thomson
S. M. Wiederhorn
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L. E. Smith, Chief
B. M. Fanconi, Deputy
Ceramics
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S. J. Dapkunas, Deputy
Fracture and Deformation
H. I. McHenry, Chief
Deputy, Vacant
Reactor Radiation
R. S. Carter, Chief
T. M. Raby, Deputy

REACTOR RADIATION DIVISION
460

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E. C. Maxwell, Admin. Officer
M. Long, Admin. Assist.
*S. E. Tassey, Secretary
S. C. Shatzer, Clerk-Typist

Neutron Radiography

- T. Cheng
- **M. Ganoczy

Division Staff

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- B. Mozer
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J. Torrence, Deputy Chief
C. Harrison, Secretary

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- F. Clark
- J. Clark
- H. Dilks
- L. Lindstrom
- M. McDonald
- W. Meuller
- T. Meyers
- J. Ring
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- R. Stiber
- A. Toth
- D. Wilkinson

ENGINEERING SERVICES

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Mechanical Design

- E. Guglielmo
- J. Sturrock
- M. Suthar

Electronics

- J. Beatty
- R. Conway
- R. Hayes

NEUTRON CONDENSED MATTER SCIENCE

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L. Roadarmel, Secretary
*L. Clutter, Clerk-Steno

rystallography

- #F. Beech
- C. Choi
- #V. Himes
- A. Mighell
- #H. Prask
- E. Prince (1/2)
- W. Rymes
- A. Santoro
- *J. Stalick

Magnetic and Amorphous Materials

- R. Erwin
- #T. Giebultowicz
- W. Knill
- #W. Li
- *J. Lynn
- J. Rhyne
- #M. Spano
- #Y. Yu
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Materials Microstructure

- N. Berk
- D. Fravel (1/2)
- C. Glinka (1/2)
- J. Gotaas
- J. LaRock (1/2)
- S. Satija (1/2)

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- D. Neumann (1/2)
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- R. Williams (1/2)
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- E. Prince (1/2)
- J. Grillo

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Cold Neutron Program

- #J. Copley
- D. Fravel (1/2)
- C. Glinka (1/2)
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- P. Kopetka
- J. LaRock (1/2)
- C. Majkrzak
- D. Neumann (1/2)
- S. Satija
- I. Schroder
- T. Thai
- T. Udovic (1/2)
- R. Williams (1/2)
- D. Pierce
- M. Rinehart

*Part-time
+WAE, Coop, Intermittent
**Deceased
#Guest Scientist, Research Assoc. (Full Time)

Research and Engineering Staff

N.F. Berk	o Condensed matter theory o SANS theory for microstructure analysis o Computer software for graphics and data analysis
R.S. Carter	o Reactor physics and nuclear engineering o Cold Source development
R.C. Casella	o Theory of neutron scattering from light-atom defects in metals o Group theory analyses of neutron scattering from condensed matter o Elementary particle theory, especially as related to reactor generated experiments
R. Conway	o Electronic engineering o Reactor instrumentation
R.W. Erwin	o Magnetic materials o Phase transformations o Spin echo techniques o Cryogenics
C.J. Glinka	o SANS microstructure of metals and porous media o Magnetic materials o Cold neutron instrument development
J. Gotaas	o Low temperature phase transformation o SANS microstructure studies o Magnetism
V. Himes	o Crystal database development o X-ray crystallography
P.A. Kopetka	o Mechanical engineering o Cold Source design o Electro-mechanical systems
J. LaRock	o Mechanical engineering o Neutron instrumentation design
C.F. Majkrzak	o Condensed matter physics o Polarized neutron scattering o Polarizing and monochromating devices
A. Mighell	o Crystallographic database development o Single crystal diffraction o Theory of crystal lattices
B. Mozer	o Structure and microstructure of metallic glasses o Dynamics of liquids o NDE of alloys

D. Neumann	o Two-dimensional materials o Solid state physics o Neutron and x-ray scattering instrumentation
J.H. Nicklas	o Mechanical engineering o Reactor fuel design o Reactor engineering support
D. Pierce	o Mechanical engineering o Neutron instrumentation design
E. Prince	o Structural properties of alloys, catalysts and minerals o Advanced crystallographic refinement methods o Software for materials structure analyses
T.M. Raby	o Reactor operations o Sample irradiations o Reactor standards
J.J. Rhyne	o Properties and transformations of high technology magnetic materials o Structure of amorphous solids o Data acquisition and analysis system
J.M. Rowe	o Orientationally disordered solids o Hydrogen in metals o Cold neutron research and instrumentation
J.J. Rush	o Catalysts and molecular materials o Hydrogen in metals o Two-dimensional systems o Inelastic scattering methods
A. Santoro	o Structure of electronic and structured ceramics o Theory of crystal lattices o Powder diffraction methods
I.G.Schroder	o Cold neutron instrumentation development o Nuclear and engineering physics o Optical devices for neutron transport
S. Satija	o Low-dimensional molecular systems o Fractal aspects of microporous media o Neutron reflectometry
J. Stalick	o Neutron and x-ray diffraction o Inorganic chemistry o Crystal database development
J.F. Torrence	o Reactor supervision o Reactor maintenance
T.J. Udovic	o Neutron time-of-flight instrumentation o Properties of catalysts o Spectroscopy of surfaces

DESCRIPTION OF TECHNICAL ACTIVITIES

The technical activities of the Division are summarized in this section. A more detailed description of each project can be found in the NBS Technical Note "NBS Reactor, Summary of Activities July 1987 through June 1988."

REACTOR OPERATIONS AND SERVICES

T. Raby

The NBSR is a national center for the application of neutron methods and standards to problems of national importance. The reactor provides intense neutron beams and sample irradiation facilities for more than 350 participants from many NBS divisions and outside organizations.

FY 88 REPRESENTATIVE ACCOMPLISHMENTS

- o Major repairs were successfully made to the reactor thermal shield cooling system.

- o Design drawings and specifications were prepared for new main reactor heat exchanges incorporating many improvements that have been developed in the industry in recent years.

REACTOR OPERATIONS AND SERVICES

T. Raby, J. Torrence, J. Ring, and N. Bickford

There were numerous activities this year that required extended reactor shutdown or operation at reduced power. Included among these are the installation of the cold neutron source, the beginning of construction of the new guide hall and confinement building annex, replacement of the shim arms, overhaul of the fuel transfer system and shipment of spent fuel. Two major problems were also encountered during this period, the failure of one of the main heat exchanger and the progressive leaks in the thermal shield cooling system. As a result, the reactor was on-line about 50% of the time at various power levels which is equivalent to about 35% had the reactor been operating at the full power level of 20 MW throughout.

Installation and testing of the cold source was a difficult and lengthy operation. The entire core was unloaded and the systems drained. The operation required almost three months. Construction of the new cold neutron facility complex was begun and is in progress. Shutdowns between operating cycles were extended to permit the contractor to do work near the confinement building. Application for license changes and associated safety analyses, to incorporate the new cold neutron guide tubes into the NBSR Technical Specifications was made to the Nuclear Regulatory Commission.

The shutdowns period was used to perform major maintenance operations. The fuel transfer system was overhauled. The shim arms were replaced for the second time after seven years of operation. The replacement took less than a month compared to nearly six months the previous time. Shipment of all spent fuel was completed. In all nine shipments were made involving 180 elements which is equal to all the previous shipments since the NBSR began operation.

A long standing problem has been leaks in the thermal shield cooling tubes. These tubes are buried inside the biological shield and are not accessible. The system consists of many redundant individual tubes with separate valves enabling leaking tubes to be isolated. At the beginning of this year, more than 50 of the 190 cooling tubes were isolated as known or suspected leakers. To address this problem we finally located a firm that has developed a method for sealing such leaks in highly radioactive environments. They were successful in sealing all but two or three of the leaks. A few have reopened during successive operating cycles, but, on the whole the results have been quite satisfactory. We anticipate that periodic treatment will continue to be required, but it appears that sound and reliable operation of the thermal shield system can be maintained at reasonable cost.

The operating staff now numbers 16, fifteen of whom are licensed senior operators, and one in training for licensure. The staff is considerably smaller than that of comparable reactors. This requires each member of the staff to carry out duties and responsibilities significantly beyond that of routine shift operation of the reactor.

A summary of the operating statistics for the past year is presented in the following table. Fuel utilization continues to be the best in the country.

No. of equivalent days at 20 MW	126
Equivalent on-line time at 20 MW	35%
Average U-235 burnup	66%
No. of irradiations	675
Hours of irradiations	1850
Hours per irradiation	2.7

The same program of reactor irradiations continued. Irradiation services were provided to many organizations from within and outside NBS covering wide areas of research, applications, and standards.

ENGINEERING SERVICES

J. H. Nicklas and R. S. Conway

In addition to normal engineering and design services provided to reactor operations, and experimenters, the engineering staff was involved in a continuing effort to upgrade the reactor systems, components and instrumentation. Among the major projects undertaken are:

New fuel elements have been qualified and are currently in production. These more heavily loaded elements will increase reactor core lifetime and will result in considerable cost savings throughout the fuel cycle, fewer shutdowns, and less handling for refueling.

For the first time, replacement shim arms were assembled with completely new mounting components. In the past, the old mounts which were highly radioactive had to be used. This required the entire assembly operation to be done remotely under water which required two months to complete. During this previous replacement, the old mounts were carefully inspected and the precise measurements needed to make new mounts were determined. The use of the new mounts eliminated the lengthy time required previously to disassemble the used shim arms from their mounts and reduced the shim-arm replacement time to less than two weeks. Because of the success of this procedure, another set of mounts was immediately fabricated for future use. For years, the fuel transfer system has been causing problems because of the sticking transfer arms due to worn out bearings that we have not been able to replace because of their location. A unique tool has now been designed and fabricated to remove and replace some of the bearings. The first attempt to remove the bearings with the new tool will be made in the near future.

The design drawings and specifications for the replacement of the main heat exchangers are in the final stages of completion. The existing heat exchangers have been the source of numerous problems, that resulted in significant loss of operating time and some loss of valuable heavy water. The new heat exchanger design will utilize advanced fabrication methods, testing procedures and new stainless steel alloys that are resistant to stress corrosion. This will assure their long life and reliable operation. A survey is being made to evaluate tube and heat exchanger manufacturers. Technical visits have already been made to several leading manufacturers across the country.

The cryogenic bismuth tip instrumentation project was completed. This instrumentation system monitors the temperature and rate of the D_2O amd H_2O cooling water flow through the bismuth tip. This project involved installing stainless steel piping, tubing, venturi flow elements, transducers, alarm units, thermocouples, analog, and digital readout meters. The entire system including safety functions and alarms, was interfaced with the reactor console control room. This allows the operator to monitor performance and take corrrective action as required. The final checkout and energizing of the bismuth tip instrumentation readout panels and alarms was completed on schedule.

NEUTRON SCATTERING CHARACTERIZATION OF MATERIALS FOR ADVANCED TECHNOLOGIES

This task develops and applies neutron scattering techniques for precise measurement and research on the structure and submicroscopic properties of industrial and high technology materials which underlie their processing and use in technological applications. It establishes and maintains a national center and state-of-the-art research facilities using neutron techniques. It also fosters the application of neutron methods to NBS programs and to serve the diverse needs of the U.S. scientific and industrial communities.

Neutron beams are a powerful probe of the critical microscopic properties of materials used in the design, development and production of industrial products, in particular new materials for advanced technologies. The neutron scattering expertise and state-of-the-art, nine-spectrometer network at the NBS reactor are a central resource for 13 NBS divisions and offices and for over 60 U.S. industries and universities (over 220 participants) which need neutron techniques to address an increasing number of problems and opportunities in materials science, physics, and chemistry. Neutron scattering provides critical information on all classes of materials, which cannot be obtained by other techniques. Neutron diffraction and radiographic methods and a materials structure database are developed and maintained to meet NIST and U.S. needs for more precise structural analysis of materials. Improved capabilities are also developed to nondestructively measure stresses and defects which affect the performance and failure of modern structural materials. Inelastic, quasielastic, and magnetic scattering methods are tailored as key probes of the submicrosopic properties of high-technology magnetic materials, industrial catalysts, and superconductors. To serve the crucial U.S. need for cold neutron measurement technology, a large cold-neutron source has been developed to be used for neutron spectroscopy and small angle scattering and ultimately to serve 15 experimental stations at the NIST Cold Neutron Research Facility.

NIST scientists are currently engaged in cooperative research with industrial labs and universities on new or improved materials for power transformers, automobiles and aircraft, sonar and microwave devices, microbatteries, high-strength polymers and ceramics, chemical catalysts, and microporous materials. Neutron methods are essential to many high priority NIST program areas, including surface science, chemical engineering, ceramics processing, and polymers and composites and high T_c superconductors. Outside interactions and cooperative materials research underway includes industrial labs (e.g., Exxon, Allied, E-Kodak, IBM, AT&T, W. R. Grace, GTE, DuPont, Bellcore), government (Army and Navy Labs, Sandia, Smithsonian), universities (e.g., U. MD., U. Illinois, U. Calif., Auburn, Notre Dame, Johns Hopkins, MIT). Joint research agreements or collaboration also in place with international centers: Institute Laue-Langevin, Saclay research centre, and CNRS (France), KFA, Jülich (W. Germany), U. Antwerp (Belgium), Chalmers Institute (Sweden). The materials structure database serves a nationwide user group from industry, universities and government, and has joint agreements with data centers around the worlds.

FY 88 Representative Accomplishments

- The D_2O ice cold source was successfully put into operation. Extensive startup tests were completed in the fall, and it has been in routine operation since December 1987. It has increased the neutron intensity available for the Small Angle Neutron Scattering and Time of Flight facilities by factors of 3 to 5.

- Atomic disorder on "plane" sites in 1, 2, 3 high T_c superconductors was found to be far more detrimental to superconductivity than disorder on "chain" sites, strongly suggesting the more critical role of the planes in the superconducting interaction. This neutron diffraction study of atomic substitutions for Cu also established the preferential occupancy of chain and plane sites according to the valency of the substituted atom.

- A systematic evaluation of the structure of the new ceramic superconductors has defined two crystallographic "building blocks" which can be arranged to reproduce the structure of all recently developed high T_c materials. These results provide a predictive tool for synthesis of new superconducting compounds.

- Recent research to exploit neutron reflection and grazing angle diffraction as powerful probes of surface and interfacial structures has produced very promising results. As an example, we have carried out (with IBM) a dramatically successful first study of lamellar formation and surface ordering in diblock copolymer films and have demonstrated the ability to measure reflectivities as low as 10^{-6}.

- During the past year neutron spectroscopic and diffraction studies of pillared clays with great potential for tailored applications in chemical catalysis and exchange have provided new insight on the orientation of pillaring ions. Direct information has also been obtained on the torsional potentials of intercalated tetramethyl ions, which provide the first experimental results to test current models of the interlayer template potential of a clay.

- Recent theoretical advances by RRD in calculating the SANS from a topologically realistic model of a bicontinuous structure have been shown to accurately describe the scattering from controlled pore glasses, thus providing a basis for using such materials to study chemical and physical processes occurring within porous media.

- Neutron diffraction results have demonstrated the existence of long range incommensurate magnetic order in the Ising-like rare earth alloy system Er-Y at Er concentration levels approaching 1%. These results reflect the very long range character of the interactions in these indirect exchange systems and unequivocally show that a spin glass state is not formed even at dilute concentrations as was presumed from conventional bulk measurements.

- In our crystal data program a new computerized electron-diffraction standard reference database has been implemented for phase characterization by electron and other diffraction methods. The database and associated software permit highly selective identification methods. The database for microscopic as well as macroscopic crystalline materials. This new database will prove a practical tool to electron diffractronists because analytical electron microscope data is precisely what is required to reliably identify and characterize unknown phases.

1. Microscopic Properties of Chemical Materials

R. C. Casella, D. Neumann, T. Udovic, J. J. Rush, W. Rymes, J. Nicol[1], and S. F. Trevino[2]

[1]Guest Scientist, University of Maryland
[2]Guest Scientist, Army Armament Munitions and Chemical Command

Catalysts and H in Metals

In our research on the vibrational dynamics and molecular motions in zeolite catalysts, we have obtained new results on differences in catalyst framework vibrations for zeolites H-Y and H-RHO. Low energy modes have been observed which are identified as proton-coupled pore opening modes of the two zeolite frameworks, which contain different external linkages and are shown to be structure sensitive. Work is in progress to investigate other systems to further correlate these low energy features with framework geometry. In addition as part of a study of the interaction of molecular hydrogen with exchangeable cations in zeolites, (with LASL and ICI) we have investigated the molecular dynamics and potential of H_2 adsorbed in CoNa-A zeolite. Neutron spectra at 12°K in the 1-40 meV range have revealed transitions at 3.8, 15.3, and 27.5 meV. The assigned rotational peaks (3.8 and 27.5) are well accounted for by a 2-fold cosine potential for the weak H_2...Co link, with a barrier height of 5.7 kJ/mole. The results also show that little dissociation of H_2 occurs even at room temperature.

In our hydrogen in metals research we have extended (with Paul Scherer Institute) our research on the novel pairing potential of protons in hcp yttrium to an analogous rare-earth metal, scandium, which also retains H in solid solution down to very low temperature. Again, similar to α-YH_x, the vibrational mode along the c-axis is both substantionally lower (30%) in energy than the basal plane modes and intrinsically broader. However no clearcut spitting of the c-axis mode due to pairing is resolved, which indicates that the short range ordering of pairs is less extended than in yttrium. Studies of the H concentration dependence are planned, along with investigation of possible non-classical hydrogen diffusion behavior along the c-axis by quasielastic neutron scattering. In another area we have completed the analysis of an extensive investigation of the vibrational dynamics and bonding sites of H in amorphous $Pd_{85}Si_{15}H_x$ by measuring neutron spectra over two orders of magnitude in H concentration (X=0.0013 to 0.08). Previous thermodynamic and diffusion experiments on this prototype system have been interpreted in terms of a Gaussian distribution of site energies, but a recent quasielastic neutron scattering study suggests a bimodel distribution of energies. The present results show the existence of two bands of H vibrations, which indicate the existence of at least two types of H sites (octahedral and tetrahedral), with octahedral type sites preferentially occupied at lower concentrations.

Two-Dimensional and Layered Materials

During the past year we have continued our work on the structure and dynamics of foreign molecules and ions which have been intercalated into layered solids. This research has centered around two particular host materials, clays and graphite.

Smectite clays are a naturally occurring class of expandable layered silicates in which two-dimensional oxyanions are separated by layers of intercalated cations. It has recently become possible to exchange the interlayer ions with a wide variety of large cations which act as "pillars" proping apart the host layers. This induces permanent porosity in these materials with a range of pore sizes and adsorption properties similar to those present in zeolites thus holding out the promise of fabricating pillared clays which have catalytic properties tailored to a given chemical reaction. In collaboration with scientists from Michigan State University and Schlumberger-Doll Research, we have performed inelastic neutron scattering experiments on the BT4 filter analyzer on trimethylammonium vermiculite and tetramethylammonium montmorillonite in order to elucidate details of the clay-pillar interaction. These results have yielded valuable information on the orientation of the pillaring ions and are now being used to refine lattice dynamical models of the clay host. In addition, the energies of the torsional modes of the methyl groups in the case of tetramethylammonium montmorillonite have shown that the clay adds about 30 meV to the rotational barrier, thus providing the first experimental information testing current models of the interlayer template potential of a clay. We have also performed small angle neutron scattering experiments on clays pillared with polyoxycations of chromium in order to determine the size and orientation of the pillars. These results have shown that the charge density of the clay layers is crucial in determining the structure of the pillars.

Work has also continued on the low temperature rotational levels of ammonia molecules in K-ammonia intercalated graphite in collaboration with scientists form the University of Illinois and the Institut Laue-Langevin. These studies have shown that a simple six-fold potential is capable of explaining the general features, but not the details, of the inelastic neutron scattering spectrum. In order to put further constraints on the model, we have performed a similar set of experiments on deuterated samples, the results of which are now being analyzed. We have also performed the first experiments which examine the stage dependence of the rotational potential of these materials in order to determine the importance of the interlayer intercalate-intercalate interaction. Finally, we have begun studies on the rotational dynamics of molecular hydrogen absorbed in potassium intercalated graphite in collaboration with scientists from Ames Laboratory and the Massachusetts Institute of Technology in order to elucidate details of the rotational potential in the incommensurate modulated phase.

2. Microscopic Properties of Magnetic, Superconducting, and Amorphous Materials

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[1]University of Notre Dame
[2]Consultant, University of Maryland
[3]Guest Scientists

This continuing effort provides a focus for the development and application of neutron elastic and inelastic scattering techniques for fundamental studies of the microscopic properties of new classes of magnetic materials (including layered magnetic systems, rare earth compounds, magnetic semiconductors, magnetic superconductors, amorphous and disordered magnetic alloys, and spin glasses.) Major new thrusts this year have included an expanded effort on the new high T_c super-conductors and cooperative study with the University of Nancy, France, on layered transition metal materials which has received a NATO grant. Much of the research on this project is carried out in collaboration with many industrial and government labs and universities.

During the year the main efforts of the project has been in (1) studies of magnetic coherence in artificial metallic superlattices involving uniaxial as opposed to planar spin configurations, (2) determination of the role of atomic disorder in "plane" and "chain" sites of the high T_c superconductor $YBa_2Cu_3O_7$, (3) determination of the antiferromagnetic ordering occurring in high T_c superconductors and its temperature dependence, (4) a first time determination of the pair-wise exchange interaction in dilute magnetic semiconductors, and (5) discovery of long-range order in dilute alloys of rare earth Er with Y and correlation with theory. The following are some of the key achievements of this research:

- The confirmation of phase coherence and the linear inverse dependence of the coherence length on thickness of a non-magnetic interlayer in rare earth artificial superlattices. The coherent effects were found to be largely independent of uniaxial or planar spin configurations found in the different rare earth metals.

- Planar antiferromagnetic order was found and its temperature dependence measured in a series of oxygen deficient $YBa_2Cu_3O_{7-\delta}$ superconductors. The ordering temperature was found to depend critically on the precise oxygen content δ and the method used to deplete the single crystals.

- Atomic disorder on "plane" sites in the high T_c superconductor was found to be far more detrimental to superconductivity than disorder on "chain" sites, strongly suggesting the more critical role of the planes in the superconducting interaction. This neutron diffraction study of atomic substitutions for Cu also established the preferential occupancy of chain and plane sites according to the valency of the substituted atom.

- Cobalt substitutions into the high T_c superconductors were found to induce magnetic order at significantly higher oxygen content than undoped materials. Distinct ordering temperatures and order parameters were also found for chain and plane sites for some compositions.

- Pair limit magnetic exchange interactions in the magnetic semiconductors ZnMnS and ZnMnSe were determined using inelastic neutron scattering in the dilute limit of less than five per cent Mn. These results represented the first such direct determination of the fundamental exchange interaction in dilute magnetic semiconductors.

- The existence of two distinct length scales in amorphous FeZr alloys was found by high resolution small angle neutron scattering. The larger of these two length scales corresponded to macroscopic static clusters or magnetic ions, while the smaller represented a limit on the spatial extent of the spin fluctuations (dynamics).

- The existence of true long range incommensurate periodic magnetic order was discovered in dilute alloys of the rare earth Er with Y down below the 3% concentration level of Er, confirming the very long range nature of the exchange interactions in these systems.

3. <u>Neutron Diffraction Methods and Applications</u>

E. Prince, A. Santoro, J. Stalick, B. Mozer, C. Choi, H. Prask[1], and F. Beech[2]

[1]Guest Scientist, Armament Munitions and Chemical Compound
[2]Guest Scientist, University of London

During the past year the study of high temperature superconductors and related ceramics has continued to be the major single area of neutron diffraction research, involving a wide range of collaboration with outside universities and industrial labs. Extensive work in collaboration with AT&T Bell Laboratories has revealed that the crystal structure of known superconducting copper oxides can be described in terms of two basic structural components (rock-salt and perovskite). These basic building blocks can be farther broken down into constituent meshes, and the structural schemes used in this description can provide a guide in the preparation of new materials with interesting electronic properties. Other research with A.T.&T. includes studies of the crystal chemistry of $La_2CaCu_2O_6$ and $La_2SrCu_2O_6$, which show a significant difference in the distribution of atoms associated with the differences in size and coordination of Ca, Sr, and La. Work has also been extended to non-stoichiometric compounds such as $YBa_2Cu_{2.7}Fe_{.3}O_{7.13}$ which suggests the existence of linear clusters of Fe cations replacing (Cu) along the [110] and [1$\bar{1}$0] directions of the tetragonal structure.

Research on "electronic" ceramics last year included studies (with the University of London) of the structure of defective pyrochlores, which support the model that the driving force in the formation of these materials is the coordination of lead (seven-fold pyramidal). These compounds are found to be primarily electronic conductors. In our research on catalytic materials, we have extended (with Dupont and Goethe University) our studies of ring ellipticity parameters affecting molecular exchange in zeolite-rho to Na and Cs-rho, which have been suggested by a previous x-ray study to show a break in the general trend which relates the lattice constant to the degree of elliptical distortion. These new results show that the x-ray results are incorrect and that the ellipticity parameter and related pore sizes do follow the previous rule. In another study (with Alfred University) we have determined the structures of highly catalytic "transitional" phases which occur during the dehydration of $Al(OH)_3$ and

AlOOH to produce α-Al_2O_3 (corundum). Work has also continued (with the Metallurgy Division and C.N.R.S., France) on N-dimensional crystallographic descriptions of icosahedral phases (quasicrystals) and their application to neutron, x-ray, and electron diffraction data on (Al, Si)-Mn quasicrystals with varying stoichiometry. Other crystallographic research (Army, University of Maryland) has included precise structure studies of cubane derivatives which have considerable interest as high density, highly strained molecules for new energetic (explosive) materials.

Finally neutron diffraction methods for residual stress and texture measurements have been applied (with Army Materials, Metallurgy, and Ceramics Divisions) to a number of materials problems. Bulk texture studies have been extended, e.g., to measurements of pole figures for cold worked depleted uranium alloys and for magnetically oriented high T_c superconductors. Residual stress studies of the failure region of 7075-T6 Al nose pieces ("ogives") for the M483 155mm projectile continued. Examination of end-items from two manufacturers--one of which produces high fail-rate ogives--identified residual stress difference consistent with the failure mode. Work in progress includes determination of the stress distributions in ogives from the high fail-rate group before and after an apparently critical cold-sizing step. New efforts have also begun to determine residual stress distributions in tantalum EFPs (explosively-formed projectiles), of great current interest to the Army, and in Ta shaped-charge liners for the Navy.

NBS Crystal Data Center

A. D. Mighell, V. L. Himes, J. K. Stalick, and M. Mrose[1]

[1]Guest Scientist, U.S. Geological Survey

The NBS Crystal Data Center is concerned with the collection, evaluation and dissemination of structure data on solid-state materials. The Data Center maintains a comprehensive database with chemical, physical and crystallographic information on all types of well-characterized substances. These materials fall into the following categories: Inorganics, organics, organometallics, metals, intermetallics, and minerals. During the year, the database and specially designed scientific software have been made available to the scientific community in three distinct modes: 1) the **NBS Crystal Data** Distribution Package; 2) International Online Search System; and 3) a new Electron Diffraction Database. Special emphasis has focused on the preparation of an update to **NBS Crystal Data** with over 20,000 entries and on the Electron Diffraction Database as discussed below.

The Electron Diffraction Database is a new computerized Standard Reference Database designed for phase characterization by electron, neutron or x-ray diffraction methods. The Database and associated software permit highly selective identification procedures for microscopic as well as macroscopic crystalline materials. Work on this new product was carried out in collaboration with the Sandia National Laboratories and the International Centre for Diffraction Data.

The Electron Diffraction Database has been designed to include all the data required to identify materials using computerized d-spacing/formula matching techniques. To permit selective d-spacing/formula matching procedures, all the required d-spacings for each material are explicitly stored in the Database. Thus in each entry, there are up to 60 interplanar spacings including all the largest d-spacings (low two theta) that are most diagnostic for identification purposes. The d-spacings are either calculated (approximately 86%) or observed. For those cases in which the cell is known, the d-spacings were systematically calculated starting with the largest d-values and ending at the cutoff value of 0.83 Å. Known space group and centering data were used to eliminate d-spacings corresponding to geometrically extinct reflections. For those cases in which the cell is unknown, observed d-spacings were used.

The Electron Diffraction Database will prove a practical tool to electron diffractionists because the experimental data obtainable from the analytical electron microscope (AEM) is precisely that required to reliably identify and characterize unknown phases. Extensive experience with searching the database demonstrates that search/match procedures based on chemistry and calculated d-spacings are extremely reliable. A knowledge of elements present and absent in an unknown is usually sufficient to give a limited set of potential candidates when searching the entire Database. Likewise experience has shown that a knowledge of low-angle d-spacings is highly diagnostic. Matching these d-spacings of an unknown against the Database also yields a limited answer set. Consequently, when these two sets (D-spacings and formulas) are intersected, the experimentalist usually obtains a relatively short, but complete, list of all compounds that could have caused the observed experimental data. Due to the quantity and quality of the reference data available in the Database, the d-spacing/formula method can routinely be used for compound identification in the analytical laboratory.

Radiographic Methods and Standards

R. S. Carter, Y. T. Cheng[+] and J. S. Olin[+]
[+]Research Associate, Smithsonian Institution

Cooperation continues with the Smithsonian Institution on the study of works of art by neutron activation autoradiography techniques. The engineering design and fabrication details have been completed for the modification of reactor thermal column area to facilitate safer, more efficient painting activation procedures and to accommodate the study of larger sized paintings. Also a new collaborative project has been started with the National Museum of American Art (NMAA) to study the works of Albert P. Ryder. His works are highly imaginative and "picture the inner reality of the mind and present to us the purest poetic imagery in the century." Nine of his paintings have been studied. The results show great contrast in style, working techniques and paint pigment usage between him and another early american artist Thomas W. Dewing. The autoradiographs provide direct, graphic records of the artist's working method and the accompanying neutron activation analysis gives the elemental composition information of the painting. The result of this study will be included in a special Ryder exhibition scheduled to open at NMAA in 1990.

We also have applied neutron activation analysis to our radiographic study of twenty-one Tibetan religious bronze figures from the National Museum of National History collection. The analysis shows that these bronzes are in general alloys of copper and lead with small amounts of arsenic and tin. The variation of copper content which ranges from about 70% to 95% indicates that there are probably multiple origins for these bronzes.

4. Materials Microstructure

Small Angle Neutron Scattering

J. A. Gotaas, C. J. Glinka, N. F. Berk, and J. LaRock

The enhanced flux at long wavelengths from the cold source was immediately exploited by users of the facility this past year to improve and extend the scope of measurements in a variety of areas. The law Q limit of the SANS instrument is now ≈.0025. As an example, G. Long (Ceramics Division) and S. Krueger (Polymer Division) measured the multiple small angle scattering from sol-gel prepared porous silica bodies that had been densified to varying degrees by sintering. Measurements over a wide range of wavelengths are needed to extract information on the pore size and number density using the theoretical framework for interpreting such data developed by N. F. Berk. By using wavelengths from t to 18 Å, the mean pore radii of samples with porosities ranging from 2 to 40% could be determined. A similar set of measurements was carried out by R.A. Page (Southwest Research Institute) on samples of sintered alumina.

The capability of reaching smaller Q-values has enhanced the sensitivity of measurements of the interaction parameter X that characterizes the compatibility between the components of a polymer blend. This capability has been used by several groups studying polymer blends including, for example, C.M. Roland and C. Trask (Naval Research Laboratory) who measured the composition dependence of X in polyisoprene/polyvinylethylene blends, J. O'Reilly and H. Yang (Eastman Kodak) who examined polycarbonate/polyester blends, and C. Han (Polymer Division) and collaborators who have studied various rubber/rubber blends and block copolymer/homopolymer blends.

In addition to this continuing work on blends, scientists from the Polymer Division have initiated several new programs involving SANS. W. Wu together with S. Roy (University of Massachusetts) have characterized the growth of clusters in polyvinyl alcohol aqueous solutions as the sol-gel transition is approached. Wu, along with co-workers from Colorado State University, has also carried out a combined SANS and SAXS study of block copolymers of alternating rigid rod and flexible polyquinoline, a candidate material for use in polymer-polymer composites. The differences in scattering contrast in these materials for neutrons and x-rays enabled the scattering from microvoids to be identified and separated from that from the polymer matrix. In another new effort, C. Han (Polymer Division) and several collaborators from Japanese Universities have carried out the first in-situ SANS measurements of polymer systems under shear. They have observed changes in the phase diagram and anisotropic scattering indicative of differences in chain conformation parallel and perpendicular to the shear directions in polystyrene/polybutadiene/solvent mixtures.

There have been a number of novel applications of the SANS technique outside of the field of polymer research as well. For example, A. Moini and T. Pinnavaia (Michigan State University) in collaboration with D. A. Neumann have initiated a study of the structural characteristics of chromia-pillared clays, a recently discovered class of microporous materials with interesting catalytic and absorption properties. They have found quite different structures depending on the host clay and have observed for montmorillonite clay, a rather well defined interpillar spacing implying a highly regular two-dimensional porous network between the clay platelets. In another novel experiment, changes in the self-organization of certain lipid chain molecules from spherical liposomes to long (up to several hundred microns) cylindrical tubules are being explored by S. Krueger and C. Han (Polymer Division) together with P. Shoen (Naval Research Laboratory). Using both contrast variation and partial deuteration of the lipid chains they are testing various models for the packing of the chains in order to gain insight into how the progression from micelles to sheets to tubules takes place.

As part of the ongoing theoretical effort in analyzing SANS data, recent advances made in calculating the scattering from a topologically realistic model of a bicontinuous structure have been shown to give a good account of the scattering observed from controlled pore glasses produced by phase separation of a binary mixture and subsequent leaching of one phase. Furthermore, it has been possible to incorporate fractal surface roughness within the framework of the model and to calculate the scattering that would be observed from such surfaces or interfaces.

One result of installing the cold source, combined with an increased awareness of the SANS facility stimulated by a workshop on cold neutron methods held in the Spring of 1988, has been an increase in requests for beam time by external groups. During any given scheduling period, requests for beam time exceed what is available by factors of two to three.

Neutron Reflectivity and Grazing Angle Neutron Diffraction

C. J. Majkrzak, D. Neumann, S. Satija

We have recently initiated a comprehensive program of neutron reflectivity measurements from surfaces and have succeeded in measuring reflectivities down to levels of 10^{-6}. The power and uniqueness of this technique has been demonstrated by measurements on thin films of block copolymers of polystrene (PS) and polymethyl methacrylate (PMMA). The experiments are a result of the collaboration with S. Anastasiadis and T. P. Russell (IBM, Almaden Research Center). Neutron reflectivity measurements on the films of PS/PMMA annealed above the glass transition temperature show a remarkable degree of orientation of the microphase separated lamallae parallel to the surface and gives detailed information about the interface between the two blocks, PS and PMMA. Properties of the diblock copolymer films are being studied as a function of temperature, molecular weight of the polymer, and various substrates (e.g., quartz, silicon, saphire, etc).

In a closely related development, the first surface diffracted neutron beam excited under glancing incident angle conditions was recently observed at the NBS reactor by an NBS-University of Illinois collaboration. The development of this new technique opens up a wide variety of studies in surface and interface physics which are difficult or impossible to perform using other methods. In particular, neutron studies of surface magnetic structures, magnetic thin films, and low atomic number adsorbates and films promise to be very fruitful lines of future research.

5. NBSR Cold Neutron Source

R. S. Carter, P. Kopetka, J. M. Rowe, J. J. Rush, D. Fravel, J. A. Gotaas

The NBSR cold source was installed in August 1987 and became operational in October 1987. The source is a 16 L block of D_2O ice maintained at 35 K with a large (8" diam.) reentrant hole. In anticipation that its performance could be improved by the addition of some H_2O, a series of tests were performed over a period of several months with different H_2O concentrations. The optimum H_2O concentration was found to be 7 1/2%. (See "Cold Source Spectrum and Flux Measurements" elsewhere in this report).

The gain in cold neutron intensity ($\lambda > 4$ Å) achieved by the cold source was determined in several ways. These included the gain relative to the best intensity that could be obtained from the best beam hole available without a cold source; the gain versus the cold source empty; and the gain versus the cold source full, but warm. The gains were 3, 5, and 10 respectively. (For more detail see "Cold Source Spectrum and Flux Measurements" elsewhere in this report).

Radiation damage studies were performed by measuring the release of H_2, O_2, and the production of H_2O_2 as a function of radiation exposure. After a specified number of megawatt-hours of operation, the reactor was shutdown and the system allowed to warm up gradually. As the system warmed, the release of D_2 and O_2 was measured. The rate of gas release as a function of ice temperature typically showed two peaks, one at ~200 K and the other near the melting point. In general most of the release was deuterium with very little oxygen. Analysis of the water after melting showed that most of the oxygen could be accounted for by the formation of D_2O_2 found in the water. As expected, based on earlier results in the literature, the D_2 released tended towards a saturation value. The D_2 releases are well within those anticipated and do not present any safety threat to the integrity of the cold source. From the figure, it is concluded that extended periods of operation pose no safety concerns. In fact, the exposure limit of the ice is set by the tritium level generated in the D_2O ice by neutron capture rather than the buildup of radiolytic products. After about twelve weeks of irradiation at 20 MW reactor power (3 reactor operating cycles), the tritium level in the cold source ice begins to exceed that in the reactor (D_2O moderated and reflected) primary cooling system. Therefore, it is deemed prudent to melt the ice after 3 reactor cycles and replace it with fresh material.

A phenomena that was not anticipated and that further limits the long term buildup of radiolytic products was the occurrence of spontaneous recombination of these products even when the ice is cold. This may be due to local hot spots that allow some recombination and energy release. This process or "burp" causes a significant fraction of the accumulated radiolytic products to recombine releasing enough energy to cause the ice temperature to rise to 80 to 90 K. Although this energy is easily absorbed in the ice, the rapid temperature rise perturbs the refrigerator which cools the ice, and may cause it to shutdown if unattended. This "burp" phenomena appears to occur about every 3 days or so at full reactor power. Therefore, every two days the ice temperature is intentionally raised by decreasing the refrigerator cooling to initiate a "burp" in a controlled fashion.

This procedure, which warms up the ice for about one hour every 48 hours, permits long term continuous operation without uncontrolled perturbation of the refrigerator cooling system.

Thus, the length of time that ice may be maintained in the cold source is not limited by the buildup of radiolytic products, but by the operational desire to limit the buildup of trituim to a readily manageable level. This requires the melting and replacement of the ice only four times a year. To assure that the ice can be maintained frozen for such long periods of time, a simple, backup refrigerator capable of maintaining the ice below freezing temperature is available on standby if the main refrigerator should fail.

COLD NEUTRON RESEARCH FACILITY

The goal of this program is to develop a world-class Cold Neutron Research Facility at the NBS reactor. This facility will include 15 new experimental stations associated with an eight beam guide tube network in a new experimental hall of dimensions 200 feet by 100 feet. Additional support space of 15000 $ft.^2$ will also be provided. Funding for this program began in FY 87 and eight new scientific, engineering and support personnel have been brought on board thus far. The total construction cost is estimated at 25 million dollars over five years.

FY 88 Representative Accomplishments

- The Cold Neutron Research Facility civil construction is proceeding well. This portion of the project is 80% complete, with beneficial occupancy scheduled for January, 1989. The number and cost of contract modifications (which arise from design changes and differing site conditions) is well below the contingency of 5%, and below the historic average for major construction.

- The neutron guide tube contract has been awarded and construction of the components is well advanced. The first neutron guides will be delivered in the spring of 1989, on schedule.

- The conceptual designs of the first five instruments to be installed in the CNRF were completed. Three of these five instruments have passed through the detailed design stage and components are being fabricated.

- A Workshop on Microstructure and Macromolecular Research with Cold Neutrons was held in April 1988, which was attended by over 125 scientists form industry, universities, and government laboratories. Participants were given presentations highlighting research opportunities in the CNRF and had the opportunity to contribute ideas to meet U.S. scientific and instrumentation needs in cold neutron research.

Construction of the neutron guide hall and office/laboratory complex was initiated in November, 1987, and is now over 85% complete, with beneficial occupancy scheduled for January, 1989. This phase of the project is on schedule and on budget.

The neutron guide tube network has been designed, and a contract has been awarded for construction of the guides. The first deliveries are scheduled for Spring, 1989, at which time installation of the first three (of seven total) guides will begin. These first three guides will be coated with isotopic Ni^{58}; a decision on the coating for the next four guides will be made early in 1989. Installation of the first three guides will allow commissioning of eight experimental stations, two of which will be the existing SANS and TOF instruments. In addition the new 30m NIST/Exxon SANS, the neutron depth profiling stations, the prompt gamma activation analysis station and the fundamental neutron physics station will be installed during 1989. The neutron interferometer and a triple-axis spectrometer are in the last stages of design, and will be installed on one of these first 3 guides. If the PRT proposal submitted for the neutron interferometer is funded, it can also be installed on this first layout.

Several other instruments are in the conceptual and/or detailed design phase, including a spin polarized inelastic neutron scattering instrument, a high resolution time-of-flight instrument, and a neutron reflectometer. These instruments will be installed in later years as they are completed. In addition, a proposal for a second 30m SANS to be built and operated as a national user facility by NSF is in the final stages of the decision process. If this is funded, it will be installed as soon as possible, either by changing the configuration of the first three guides or on one of the next four guides.

Conceptual design of a second cold source is now underway, using neutron moderator calculations to optimize the final choice. If possible, (subject to NRC approval) this new source will be installed at the same time as the last four guides, thus minimizing radiation exposures and reactor down-time.

Considerable progress has been made on general neutron instrumentation R&D, including development of new neutron polarizers and super mirrors, neutron reflectometry,* and a comprehensive set of simulation codes for instrument design.

*A new method for chopping neutron beams to decouple slit size from resolution.

INDEPENDENT PROGRAMS

The two major independent (non-collaborative) Bureau programs using the reactor are nuclear methods group in the Center for Analytical Chemistry and standard neutron fields for neutron flux calibration and materials dosimetry in the Center for Radiation Research. These programs will be summarized here. The major non-NIST independent programs were summarized in the RRD Annual Report.

FY 88 Representative Accomplishments

- o Scientists in the Nuclear Methods Group in collaboration with NIH have determined chromium at sub ppb levels in whole-human blood, serum and packed cells. These results may have important implications for understanding the suspected important role of low level chromium in diabetes.

- o A cooperative agreement between NIST and Westinghouse is being negotiated to review the measurement techniques for power reactor neutron dosimetry used by Westinghouse to insure that direct measurements links exist with standard neutron fields at NIST.

- o NIST in collaboration with scientists from the Quantum Metrology Division, the University of Sussex, and the Central Bureau of Nuclear Measurements has undertaken an ambitious program to improve previous measurements of the neutron lifetime.

1. Nuclear Methods Group: Overview

R. Fleming

The development and application of nuclear analytical techniques for greater accuracy, higher sensitivity and better selectivity are the goals of the Nuclear Methods Group. A high level of competence has been developed in reactor-based activation analysis, which includes instrumental and radio-chemical neutron activation analysis (INAA and RNAA), as well as fast neutron activation analysis (FNAA). In addition, the group has a unique capability in neutron beam analysis with both prompt gamma activation analysis (PGAA) and neutron depth profiling (NDP). The NDP technique utilizes prompt charged particle emission to determine elemental distributions within the first few micrometers of a surface while the PGAA technique utilizes prompt gamma-ray emission to measure the total amount of an element in a sample, regardless of its distribution. These techniques provide an arsenal of tools to address a wide variety of analytical problems in science and technology.

The activities of the past year have been highlighted by the initiation of the National Facility for Cold Neutron Research to be established at NBS during FY89. The Group's involvement includes the design and construction of second generation instruments for PGAA and NDP. A major grant from the Eastman Kodak Company is contributing to the timely development of NDP using cold neutrons. In addition a facility is envisioned at which we will study the techniques for focusing neutron beams to increase the neutron intensity on a point. The combination of intense focussed beams applied to the existing analytical methods could result in greatly enhanced measurement capability.

The Group's contribution to the certification of Standard Reference Materials is illustrated by the multielement measurements done on the SRM Bovine Serum, Buffalo River Sediment, and glass-film XRF standards. A new ability to quantify nitrogen in biological samples will result from this year's research to develop an NAA- liquid scintillation beta counting method exploiting the thermal neutron reaction $^{14}N(n,p)^{14}C$ and measuring the radioactive CO_2. This project is being done in collaboration with the University of Illinois.

The Group has taken an active role in the Bureau's program on high-temperature superconductivity, both in the measurement of impurities in starting materials and in final products, and in the determination of the actual stoichiometry of the metallic constituents. The effort this year has been in the development of accurate, rapid measurements of these materials by both NAA and PGAA.

The Biomonitoring Specimen Bank Research Project continued its support for other agencies' monitoring programs. These included the EPA human liver project, the NOAA National Status and Trends program, the NCI Micronutrient program, the IAEA/NBS/FDA/USDA Total Diet Study, and most recently, the NOAA Alaska Marine Mammal Project. Research has centered on banking protocols and improved analytical methodology. Our participation in intercalibration exercises with the project participants and the development of marine QA materials helped enhance the quality of the analytical results used in the assessment of the Nation's environmental health.

Bioanalytical research focused on the determination of metal species in various materials. Elements at trace and ultratrace levels have been determined in separated proteins and other macromolecules. The use of autoradiography to determine selenium has been added to the INAA and RNAA techniques. The occurrence of inorganic and organic compounds of tin in marine tissues is also being studied.

The strong interaction with industrial scientists using neutron depth profiling, prompt gamma activation analysis, and neutron activation analysis has continued with a growing number of guest workers, research associates, and joint publications. An important development this year has been the demonstration of two-parameter, coincidence spectroscopy for thin samples in collaboration with the group under Professor W.-K. Chu at the University of North Carolina and with Eastman Kodak. For appropriate samples this technique will increase the measurement sensitivity equivalent to a ten-fold increase in reactor neutron flux.

The joint NBS/FDA/USDA study of trace elements in human diet, sponsored by the International Atomic Energy Agency, has completed its fourth year. A total of 40 minor and trace elements have been measured on the U.S. total diet material collected from several regions. In addition, measurements have been carried out on selected elements in diets received from countries participating in this global study.

During the coming year the group will continue to improve the accuracy, productivity and sensitivity of nuclear methods as applied to elemental measurements. Problems to be addressed include those inherent in sample preparation, irradiation, radiochemical separation, counting and data reduction, with the goal of minimizing and quantifying the various sources of random and systematic errors in analysis by nuclear methods.

2. <u>Neutron Interactions and Dosimetry Group</u>

J. Grundl

The Neutron Interactions and Dosimetry Group develops and applies well-characterized neutron fields and related capabilities for neutron dosimetry methods evaluation and standardization, for detector development and calibration, and for reaction cross section measurements. Strong involvement with outside organizations, both in the federal and private sectors, includes many types of research and technology assistance programs as well as leadership roles on national and international standards and radiation policy making bodies.

A selection of accomplishments for FY-88, with emphasis on NBS reactor related activities, are outlined below in titled paragraphs. Projects that define the group's activities and major participants are included.

<u>Dosimetry For Material Performance Assessment</u>

Dosimetry methods for monitoring the degradation of materials in high fluence neutron exposures are diverse. This project provides some form of measurement assurance, standardization, or methods development for nearly every approach to materials dosimetry employed in the United States. Interlaboratory measurement cooperation, including substantial European participation, are an important feature of this project.

1. <u>Neutron Fluence Standards</u>. These unique artifact standards are neutron sensors (activation foils generally) in which a radioactive species relevant for dosimetry is induced by irradiation in a standard neutron field. The National Institute for Standards and Technology (NIST) maintains a variety of such neutron fields to supply neutron fluence standards to customers under NIST SP 250 Calibration Services and to the Nuclear Regulatory Commission under a general consultation contract. These fluence standards provide benchmark referencing for dosimetry measurement methods used in the nuclear industry.

2. <u>NBS-Westinghouse Cooperative Agreement</u>. In a move to improve Quality Assurance (QA) methods associated with dosimetry procedures at commercial power reactors, NIST and Westinghouse have begun negotiating a cooperative agreement. Under this agreement, NIST will review the measurement techniques for reactor neutron dosimetry at Westinghouse to insure that direct measurement links exist with standard neutron fields at NIST. Westinghouse and NIST personnel have met and agreed upon important elements of a written agreement.

3. Dosimetry Benchmarking for the HSST-Program. NIST is helping the NRC benchmark fast neutron dosimetry for an HSST steel testing program carried out by the Materials Engineering Associates (MEA) Corporation at the University of Buffalo's Pulstar Reactor. The focus of this activity is radioactive counting procedures at the Idaho Nuclear Engineering Laboratory (INEL) where analysis of all dosimetry involved in the MEA tests are performed. Comparisons of experimental dosimetry with neutron transport calculations were presented by NIST at the 14th ASTM- E10 Radiation Effects on Materials Symposium, in Andover, MA in June 1988.

4. Fission Spectrum Cross Section of $^{93}Nb(n,n')^{93m}mNb$. Because of its long half life (16 years) and a low energy threshold (1 MeV), the Nb(n,n') reaction is a candidate for long term neutron fluence monitoring. One drawback has been the lack of adequate cross section information. Now, in cooperation with the universities of Illinois and Arkansas, the spectrum averaged cross sections of the niobium reaction have been measured in the ^{235}U and ^{252}Cf standard fission neutron fields at NIST. Free-field neutron fluences at both irradiation facilities were established by neutron source emission-rate calibrations at the NIST $MnSO_4$ Bath Facility.

Personal Dosimetry

Standard neutron fields are developed and applied for calibration of radiation protection instrumentation and for the investigation and testing of new types of dose measuring techniques. Substantial responsibilities in national and international dosimetry methods research focuses on tissue dose modeling and tissue equivalent proportional counter measurements.

1. Performance Tests of Radiation Protection Instrumentation. In a joint project involving Harwell and the National Physical Laboratory in England, and the Naval Surface Warfare Center and Naval Research Laboratory in the United States, the properties of the new Chalk River "Bubble Damage Detector" were investigated. The results of this work were sufficiently promising that this collaboration will continue under the auspices of the Naval Medical Command.

   In a separate effort to understand the cause of the persistent slow drift in the 9" remmeters commonly used for neutron radiation protection measurements, a detailed study was made of the behavior of the 3BF proportional counters used as neutron detectors in these instruments.

2. Tissue Equivalent Proportional Counter (TEPC) Studies. In a joint program with PTB and the University of Saarlands, a detailed study was made of the behavior of various configurations of TEPC's in the NIST filtered neutron beams. The purpose of this investigation was to learn how to improve the response of TEPC-based remmeters in the keV-to-100 keV neutron energy range. These types of remmeters are under active development at several laboratories in the United States and in Europe. It is recognized, however, that their performance needs to be improved in the energy region made accessible by our filtered beams.

3. International Standards Writing. The ISO Draft Standard Proposal, "Procedures for Calibrating and Determining the Energy Response of Neutron Measuring Devices Used for Radiation Protection," has been completely rewritten although further changes will have to be made. A draft of the chapter on calibrations, for the forthcoming ICRU publication "Determining of Dose Equivalents from External Radiation Sources - Part 3," has also been completed.

Research and Technology Assistance

Research activities and technology assistance are strongly coupled especially in neutron dosimetry. A multiplicity of institutional involvements, drawn to the group by unique irradiation facilities and measurement capabilities, encourages a variety of attractive projects and unavoidable responsibilities.

1. Neutron Lifetime Measurement. In collaboration with scientists of the Quantum Metrology Division, the University of Sussex, and the Central Bureau for Nuclear Measurements, an ambitious experimental program has been undertaken to improve previous measurements of the free neutron lifetime. The first lifetime data from this collaboration are expected between late August and early December, 1988 from measurements at the Institut Laue-Langevin cold neutron guidehall in Grenoble, France. The experiment will next move to the new cold neutron guidehall at NIST for more exhaustive measurements.

2. Capture Cross Section Measurement in ISNF. Spectrum-averaged cross sections for six reactions of interest in reactor physics have been measured in the Intermediate Energy Standard Neutron Field (ISNF). The ISNF neutron energy spectrum, with less complexity, resembles a fast reactor spectrum.

3. Fission Chamber Monitors at AFRRI. Neutron dosimetry at the Armed Forces Radiobiological Research Institute's reactor exposure room was put on a more stable basis by the installation and testing of two fission chamber monitors designed and built at NIST. Linearity tests of reactor instrumentation, vs. NIST absolute fission chambers and tissue-equivalent ionization chambers were carried out over the full range of reactor power at the main AFRRI Triaga exposure room.

4. Reactor Beam Calibrations. Absolute fission chambers and fissionable isotope mass standards were employed to determine absolute neutron fluence rates and improvement in the "capture flux" resulting from installation of the Cold Source at the NIST Research Reactor. These results influenced plans for further upgrading of the Cold Source.

5. Mass Assay of Ultra-Light Fissionable Deposits. Westinghouse Research Center, Pittsburgh is working cooperatively with NIST to establish mass scales for ultra-light fissionable deposits. These deposits, with masses in the picogram or sub-picogram range, are used with mica Solid Track Recorders (SSTR's) and represent a significant new dosimetry measurement technique. Currently achieved accuracy is better than five percent; The goal is three percent or better.

6. LiF Chip Development and Application. A lithium fluoride crystal dosimeter package was returned to NIST after irradiation through a full fuel cycle in the cavity surrounding the reactor vessel at the Oconee 2 nuclear power plant. The sample retained virtually perfect optical quality, despite the heat and humidity of the environment. The gamma dose recorded was comfortably within the accurately readable range. This gamma dose data will be employed by the operating utility to confirm calculations of gamma and neutron dose as they affect reactor vessel embrittlement and safe operating lifetime.

Irradiation and Calibration Facilities

Well-characterized neutron fields are built and maintained as permanent irradiation facilities providing certified fluences of pure fission neutrons, sub-MeV distributions, monoenergetic keV beams, and thermal neutrons. Passive and active detectors of all kinds are exposed in these neutron fields for response calibrations, for cross section measurements, and for the investigation of new measurement techniques. A high intensity, neutron-driven gamma field operates for special purpose measurements.

A multi-purpose fission rate measurement capability is centered around the NIST "go anywhere" double fission chambers and the NIST set of fissionable isotope mass standards (FIMS). The Manganous Sulfate Bath is the primary neutron source strength calibration facility for the U. S. Absolute neutron fluences for all fission-neutron-driven standard neutron fields at NIST are derived from source strength calibrations at this facility.

1. Cavity Fission Source Operations. Efforts to improve cavity fission source operations and calibration base documentation are continuing. A new general purpose shield cave for high and intermediate level radioactive components has been designed and shop work on the shield walls has begun. When complete, this shield cave will greatly simplify irradiation operations at the reactor thermal column.

2. Scattering Corrections in the Cavity Fission Source. Corrections for neutron scattering in the hardware and irradiation samples of the cavity fission source are under review. Existing corrections are based on Monte Carlo calculations made by LANL for an earlier configuration of the cavity fission source with a different Cd box and Al enclosure.

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Industrial and Academic Interactions

As a national center for the development and application of neutron methods in condensed matter and materials science, chemical analysis and radiation standards, the Reactor Radiation Division and other NIST organizations have direct interactions and cooperative programs with 45 universities, 22 industrial and 23 foreign laboratories. A few examples of the many interactions of the Neutron Scattering Group are:

- An agreement is in place between NBS and Exxon Research and Development Corporation to jointly develop and operate a world-class small angle neutron scattering spectrometer at the NBS cold neutron source. Active design and construction of this facility is well underway. Cooperative research efforts on the existing SANS instrument at the reactor include work on wetting in microporous media and micellar systems.

- An intense cooperative research effort was organized early in 1987 with several groups at AT&T Bell Laboratories on the systematic studies of the structure and properties of the new class of high-temperature superconductors. This joint research continues to grow and produce important new results.

- The Reactor Radiation Division's Crystal Data Center is engaged in a number of interactive links including joint development and distribution to U.S. science and industry of evaluated crystal data with the International Center for Diffraction Data. The Data Center also has long-term agreements in place with crystal data programs in Canda, Great Britain, and Germany to jointly develop and share critical data on the structure of materials. An expansion of database activities into electron diffraction and microscopy has recently been achieved.

- The Neutron Scattering Group has in place wide collaborative research with the University of California (Santa Barbara) involving neutron inelastic scatttering, neutron diffraction, and SANS studies of catalysts, non-linear optical materials, and radiation damage.

- Extensive cooperative research efforts with the Physics Department and Materials Research Laboratory at the University of Illinois and with Michigan State have continued during the past year to include neutron diffraction studies of a new class of layered magnetic materials and research on new kinds of metal-molecular complexes created within the layers of pillared clays and oriented graphite. Joint NIST/Illinois efforts have recently been extended to use of near-grazing angle neutron diffraction in surface structure studies.

- Cooperative Research Program with the Department of Physics and Astronomy of the University of Maryland. Under this program RRD staff are engaged with Maryland scientists in joint research on magnetic materials, superconductors, catalysts, and biological materials. Some of this research is carried out jointly with scientists from industrial labs.

- An extensive collaborative research effort was initated with Bell Communications Research this past year focussing on magnetic substitutions and interactions in high T_c superconductors. Associated research is also underway with Johns Hopkins on the effect of atomic substitution on superconductivity.

Associated Activities

During the past year scientists inthe Reactor Radiation Division delivered over twenty-five invited lectures in the U.S. and abroad. The Division also hosted a "Workshop on Microstructure and Macromolecular Research with Cold Neutrons" with some 160 participants. Neutron Scattering Group scientists have also received along with French and German colleagues, several NATO grants to stimulate cooperative research in such areas as magnetism and hydrogen in metals.

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This report summarizes all those programs which depend on the NIST reactor. It covers the period from October 1, 1987 through September 30, 1988. The programs range from the use of neutron beams to study the structure and dynamics of materials through nuclear physics and neutron standards to sample irradiation for activation analysis, isotope production, radiation effects studies, neutron radiography and nondestructive evaluation.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

Activation analysis; crystal structure; diffraction; isotopes; molecular dynamics; neutron; neutron radiography; nondestructive evaluation; nuclear reactor radiation

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