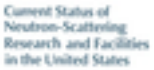

Current Status of Neutron-Scattering Research and Facilities in the United States

Panel on Neutron Scattering, Solid State Sciences Committee, Board on Physics and Astronomy, National Research Council

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Panel on Neutron Scattering
Solid State Sciences Committee
Board on Physics and Astronomy
Commission on Physical Sciences, Mathematics, and Resources
National Research Council

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PANEL TO ASSESS THE CURRENT STATUS OF FACILITIES AND RESEARCH IN NEUTRON SCATTERING

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BOARD ON PHYSICS AND ASTRONOMY

COMMISSION ON PHYSICAL SCIENCES, MATHEMATICS, AND RESOURCES

PREFACE

In the spring of 1983, the Solid State Sciences Committee, in implementing one of a series of studies addressing the health of this discipline, called together a group of experts to assess the present status of U.S. facilities and capabilities in the field of neutron-scattering research. The Panel was also asked to review recent trends in the U.S. neutron-scattering user community and to identify critical gaps in U.S. capabilities in this field with respect to those abroad. The Panel was charged to address primarily applications of neutron-scattering techniques in the condensed-matter, chemical, and biological sciences. It should be noted that a number of other critical scientific and technological areas (some of which are listed in Chapter 3 of the report) require the use of high-performance neutron sources. It is clear that these applications will have important implications in any discussion of the design and utilization of neutron sources in the future.

The Panel concluded that the United States has fallen behind Western Europe in the use of cold neutron beams and high-resolution spectroscopy. U.S. reactors remain world class in terms of neutron-beam intensities, but the United States lags in the development of new instrumentation on the reactors. An additional problem is that they are aging. Existing sources will be 20 to 25 years old by 1990. The long-range implications are serious with respect to many fundamental new applications of neutron-scattering research in the materials-related disciplines, including those of technological importance.

The Panel's report stresses the need for an immediate U.S. commitment to the development and installation of state-of-the-art instrumentation at our present research reactors; for support to permit full investigation and development of pulsed sources; and to begin planning for the next generation of neutron sources. The Panel emphasized the importance of involvement of the user community in all stages of planning of new facilities.

The Solid State Sciences Committee unanimously endorses the Panel's conclusions and recommendations. We urge the federal research agencies to move as quickly as possible to strengthen U.S. capabilities in this highly competitive and technologically promising field of research.

William F. Brinkman, Chairman
Solid State Sciences Committee

CONTENTS

1.

CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

1. In the last decade neutron-scattering research worldwide has shown a rapid expansion both in the number of users and in the diversity of disciplines and science to which neutron methods are being applied. This growth is due to the development of improved sources and new instruments, which have greatly enhanced the energy and wave-vector range, resolution, and sensitivity of neutron instrumentation. The neutron-scattering community in Europe more than tripled during the 1970s. By comparison, the U.S. community has doubled over the past 6 years, accompanied by a 150 percent increase in users from less-traditional areas--polymers, biology, and materials science.
2. In spite of some recent progress, the United States has fallen far behind Western Europe in the development of advanced facilities at research reactors, including modern applications of cold sources and guide-tube technology, focusing monochromators, and spin-echo and backreflection techniques. These advances have led to many fundamentally new applications of neutron scattering, which touch on all materials-related disciplines, including technologically important areas. The United States has maintained its competitive position and tradition of excellence in such areas as thermal-neutron triple-axis spectroscopy and chemical

and biological crystallography and, for the present, is at the forefront in pulsed-source research.

3. Current U.S. reactors remain world class in terms of available thermal-neutron-beam intensities, and there are immediate opportunities to achieve an internationally competitive status in advanced instrumentation for both cold and thermal neutron scattering at a cost substantially lower than the recent European expenditures. Such modern facilities, combined with emerging applications of pulsed-neutron sources, would stimulate greatly expanded use of neutrons to meet new scientific and technological needs and opportunities until new-generation sources are developed. It should be noted that existing sources will be 20-25 years old by 1990.

RECOMMENDATIONS

1. The Panel recommends that an immediate commitment be made to develop new state-of-the-art instrumentation at our high-performance research reactors to provide world-class capabilities in such areas as high-resolution and high-sensitivity neutron spectroscopy, small-angle scattering and diffraction, medium-resolution macromolecular diffraction, and diffuse scattering. This will require the extensive development and application of modern cold-source and guide-tube technology, focusing and polarizing monochromators, and area detectors.
2. The Panel recommends that adequate support be provided to allow full investigation and development of new pulsed-source instrumentation required to exploit the unique opportunities in condensed-matter research provided by the

pulse structure, higher fluxes of epithermal neutrons, and expanded wave-vector range of spallation sources.

3. The Panel considers it essential that serious design efforts be started immediately for the development of next-generation sources, so that definite proposals are available by fiscal year 1988. The results of such efforts are essential as input to a broadly based user group, which should be established to recommend a coherent plan to meet the longterm neutron research needs of the scientific community. It is the view of this Panel that the National Academy of Sciences-National Academy of Engineering would be the most appropriate body to establish such an independent multidisciplinary advisory group.

2.

INTRODUCTION

The development of neutron-scattering facilities and research applications worldwide has shown dramatic growth and change during the past decade. The most notable example of these changes is found in the emergence of the British/French/German Center at the Institut Laue-Langevin at Grenoble, but its development is only part of a major transformation of the field that has occurred throughout Western Europe and more recently in the United States and Japan. Over the past 25 years the unique characteristics of the neutron as a probe of condensed matter has transformed much of our fundamental understanding of the physics and chemistry of materials. In the last decade a new generation of cold and thermal neutron instruments has been developed (particularly in Europe) that has extended the wave-vector range and energy resolution for neutron experiments by orders of magnitude. These in turn have opened up new research in physics and chemistry and have greatly expanded the application of neutron scattering in new areas--materials science, polymers, and biology. For example, the neutron-scattering community in Europe has tripled in the past decade, and, more recently, there has been a great increase in the size of the neutronscattering community in the United States. Moreover, in the past few years the development of higher-intensity pulsed neutron sources has also created new opportunities for neutronscattering research using higher neutron energies. The impact of these emerging neutron-research opportunities

on U.S. science has been addressed by two reports over the past 6 years: the NAS-sponsored study, Neutron Research on Condensed Matter in 1977 and the Report of the Review Panel on Neutron Scattering, sponsored by the U.S. Department of Energy (DOE), which in 1980 presented a study of U.S. neutron-research capabilities centered around priority recommendations for neutron facilities of the DOE. We refer the reader to these earlier studies for a detailed review of the unique role of the neutron as a probe of materials. Both of these reports emphasized the much greater investment and facility advances that were being made in overseas neutronscattering research and recommended steps to be taken to assure an internationally competitive position for the United States in neutron scattering. While some of these recommendations have been addressed at least in part, most have not, and total funding has shown little change in real dollars over the past 6 years. The present study is the response to a request by the Solid State Sciences Committee of the National Research Council, and attempts to provide an objective up-to-date assessment of the current status of U.S. research accomplishments and capabilities in this fast-moving field, including a review of recent trends in the American neutron-scattering user community. Critical gaps in U.S. neutron-research capabilities with respect to modern facilities at other international centers are also highlighted.

3.

CURRENT STATUS OF NEUTRON-SCATTERING FACILITIES IN THE UNITED STATES

In this chapter we describe briefly the existing neutron-scattering facilities at the five National Laboratory neutron sources and two major university reactor facilities. We also provide a summary of the trends in users and publications associated with U.S. neutron facilities. In Chapter 4 we provide a comparison with facility development and user trends at foreign laboratories.[1] It is clear from these data that there has been a striking increase in users and change in user patterns over the past decade along with

[1]A variety of sources of information were used by the Panel in assembling summaries of users, publications, instrumentation, and total neutron-scattering budgets. These included the earlier National Academy of Sciences and Department of Energy reports cited in the Introduction, the Annual and special reports of the DOE and its National Laboratories, the National Bureau of Standards, and the University of Missouri, along with those of the Institut Laue-Langevin at Grenoble and other neutron-scattering centers in Europe. The Panel went further, however, to assure upto-date suitably coordinated information and statistics by individually contacting the major neutron centers in the United States, Western Europe, Japan, and Canada concerning users, publications, and other information relevant to the comparisons made in the report. It should be noted that the Panel did not attempt to provide similar comparisons with neutron-scattering facilities in the Soviet Union, Eastern Europe, India, or other neutron efforts worldwide. A summary of these facilities can be found in the earlier NAS and DOE reports mentioned above.

qualitatively new research opportunities in a variety of fields.

It should be noted that in general U.S. neutron sources also serve a wide variety of scientific and programmatic needs that are unrelated to neutron-scattering research. At present, about half of the total operating costs of major neutron sources (about $13.5 million) are associated with neutron scattering, while the remainder is related to other highly important and diverse national needs, including isotope production, chemical trace analysis, radiation damage, nuclear physics, ultracold neutron research and radiation standards. This multiple program use of neutron sources in the United States is beneficial, since it can provide broad-based support and cost-effective operation. However, it can sometimes create serious difficulties if one of the programs loses or withdraws support, thus threatening the stability or schedule of source operation.

The major neutron sources in the United States used for scattering research are briefly described in the following summaries. The research reactors in general operate 24 hours a day in a quasi-continuous schedule with brief shutdowns for maintenance and refueling. The pulsed-source schedules are currently more curtailed, as noted in the summaries.

FACILITY DESCRIPTIONS

High Flux Beam Reactor (HFBR)--Brookhaven National Laboratory

The High Flux Beam Reactor is a 60-MW reactor using enriched fuel and D_2O as a moderator and primary coolant. The core

is small (48-cm diameter), resulting in a thermal neutron density that is peaked outside of the core, where beam tubes tangential to the core provide neutron beams with low fast-neutron contamination. The thermal flux is 1×10^{15} neutrons/cm^{2}sec at the 8-cm-diameter thermal beam-tube tips. To provide intense beams of low-energy neutrons, a liquid H_2 moderator has been installed in one beam tube that is equipped with a small-angle scattering diffractometer and a high-resolution three-axis spectrometer. Situated on the seven remaining tangential beam tubes are four conventional three-axis spectrometers that are used mostly for inelastic scattering studies and powder diffraction, a three-axis spectrometer and two diffractometers equipped with four-circle goniometers for single-crystal and protein diffraction studies, as well as two additional diffractometers used mainly for small-angle scattering. Four diffractometers have position-sensitive detectors. One of the three-axis spectrometers is often devoted to polarized neutron studies. Under a cooperative development are a new polarized-beam crystal spectrometer with a spin-echo capability (with Japanese scientists) and a medium-resolution macromolecule diffractometer (with Exxon Research Laboratories). Additional ancillary equipment, including conventional and ^{3}He cryostats and high-pressure sample environments are routinely available. Staff scientists carry out independent research programs in addition to assisting external users, who make collaborative arrangements largely through direct contact with interested staff scientists. A more formal user policy including peer review will be implemented in the near future.

Intense Pulsed Neutron Source (IPNS)--Argonne National Laboratory

The Argonne Pulsed Neutron Source produces bursts of neutrons with a peak thermal flux of ~4×10^{14} neutrons/cm^2-sec at a repetition rate of 30 Hz and is at present the most intense pulsed source in the world. Neutrons at the IPNS are produced by a 450-500 MeV proton-beam incident on a depleted uranium target at an average current of ~12 μA. A polyethylene moderator surrounds the target to reduce the energy of the neutrons to allow neutron-scattering research. Twelve horizontal and two vertical beam holes surround the moderator assembly. A cold moderator (80K) is available for three of the beams. A separate uranium target is used for fast-neutron irradiation and arranged so that the samples can be irradiated at liquid helium temperature. IPNS currently operates 6 months a year. The radiation effects facility receives the beam 25 percent of the time, and the neutron-scattering target 75 percent of the time.

There are seven instruments currently available in the user mode, including two high-resolution powder diffractometers; a single-crystal diffractometer operating on the Laue principle with a position-sensitive detector of the scintillation type; a small-angle diffractometer, also with a position-sensitive detector; a crystal-analyzer spectrometer primarily for observing H-modes in chemical systems; and two chopper spectrometers with incident energies ranging from 50 to 1000 MeV, which allow scattering measurements over a broad range of energy and wave-vector transfer. These neutron-scattering instruments are scheduled in the “user” mode, i.e., allocation of 75 percent time is made

by a Program Committee, which reviews proposals twice a year. Three additional instruments are under development: a polarized neutron instrument for studying refraction from surfaces; a diffractometer built to search for ordered nuclear moment arrangements in ^{3}He below 1 mK; and a spectrometer for spectroscopy in the electron volt range.

Accelerator modifications and installation of an enriched uranium target are planned over the next 2 years to increase significantly the intensity of IPNS.

Massachusetts Institute of Technology Reactor (MITR)

The MITR is a 5-MW, heavy-water moderated reactor whose core and beam arrangement was modernized in the 1970s to provide beam tubes with accessible fluxes approaching 10^{14} neutrons/cm^2-sec. There are currently three two-axis spectrometers in use, one with temperature stability control for neutron interferometer studies and two for general-purpose diffraction with changeable monochromators and wavelengths. The MITR is also utilized for a variety of other research and applications in nuclear engineering, trace analysis, radiation effects, and isotope production.

National Bureau of Standards Reactor (NBSR)

The NBSR is a heavy-water-moderated research reactor currently operated at 10 MW and awaiting final Nuclear Regulatory Commission approval to double the power to 20 MW, which will provide a flux at the beam-tube entrances of 2×10^{14} neutrons/cm^2-sec. The NBSR has eleven radial beams (15cm diameter), nine of which are currently dedicated to neutron-

scattering research. The reactor geometry combines a split-core fuel arrangement and large vertical divergence (~100 min) to provide high-intensity, low-background beams at the sample position for scattering applications. The facilities available for diffraction include a multiple-detector high-resolution powder diffractometer; a four-circle single-crystal diffractometer; a biological crystallography station (NBS-NIH) using a position-sensitive detector; a small-angle-scattering spectrometer that features a focusing collimating system, tunable wavelength (4.5-12 Å), and a large (65 cm × 65 cm) position-sensitive detector that can be rotated around the sample. Instruments for inelastic scattering include three variable-incident energy triple-axis spectrometers, one of which is equipped with a high-intensity beryllium filter analyzer for chemical spectroscopy, and a multidetector time-of-flight crystal-chopper spectrometer with variable incident energy. A polarized-beam spectrometer is also under development. Scattering experiments are possible between 0.3 and 1800 K and at magnetic fields up to 7 T. All neutron-scattering instruments are scheduled each month by a committee of major users from the National Bureau of Standards, other federal laboratories, and universities. External requests for facility use can be addressed to committee members or to the neutron group leader.

Funding has recently been provided for installation of a large (25-cm-long, 36-cm-diameter) cold-neutron source in the reactor core, which will serve a variety of instruments for cold-neutron research on materials.

Sixteen other facilities at the NBSR serve research and applications in chemical trace analysis, radiation standards, nuclear physics, and isotope production.

Oak Ridge National Laboratory Reactors (ORNL)

The High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory operates at a power level of 100 MW. Light water serves as coolant and moderator in the annular fuel region. Target rods for production of transuranium isotopes are located in a central flux-trap region. There are four horizontal beam tubes of 10-cm inner diameter with an average flux of 1×10^{15} at their tips. These beams deliver neutrons to nine scattering instruments: two variable incident energy (E_0) triple-axis spectrometers; a fixed E_0 triple-axis unit; a polarized-beam triple-axis spectrometer; an ultrasonically pulsed time-of-flight instrument; a liquid diffractometer; a four-circle, single-crystal diffractometer; a double perfect-crystal small-angle scattering (SANS) instrument; and a 30-m SANS facility with an area detector. The last instrument was constructed with NSF funds and is operated by the National Center for Small-Angle Scattering Research. A new high-intensity two-axis diffractometer with a curved position-sensitive detector is being developed with Japanese support with a potential for real-time crystallographic studies.

The Oak Ridge Research Reactor (ORR) operates at 30 MW with light water as coolant and moderator and beryllium as reflector. The primary purpose of this reactor is for materials-irradiation experiments, but there are six horizontal beam tubes of 17-cm diameter for scattering experiments. The thermal flux near the beam-tube entrances is about 2×10^{14} neutrons/cm^2-sec. The Ames Laboratory operates three instruments at the ORR: a variable-E triple-axis diffractometer, a polarized-beam diffractometer, and a two-axis diffractometer.

In addition, ORNL operates a 5-m SANS instrument with an area detector and a two-axis diffractometer.

Proposals for the NSF-supported SANS facility are reviewed by a special committee and scheduled as they are received; there is normally a three- to four-month waiting period. Other ORNL instruments are available to users either by informal arrangements or by written proposals that are reviewed by Oak Ridge staff members.

University of Missouri Research Reactor (MURR)

MURR is a 10-MW pressurized-water, beryllium-reflected fluxtrap reactor located in Columbia, Missouri. There are six beam ports with four used for neutron-scattering research. The flux available at the source end of the beam ports is 10^{14} neutrons/cm^2-sec. There are currently seven neutron-scattering instruments: two four-circle single-crystal diffractometers; one triple-axis spectrometer; two powder diffractometers--one with a position-sensitive detector, the other with a five-detector system; a fixed-wavelength (4.7 Å) small-angle scattering facility that uses a multidetector and has 4.5-m flight paths before and after the sample; and a double-crystal monochromator-interferometer instrument. Facilities are open to outside users by informal arrangem ents with neutron-scattering staff members at MURR.

The reactor has a number of other major facilities used for gamma-ray scattering (diffraction, quasi-elastic scattering, and Compton scattering), neutron activation analysis, radio-pharmaceutical and transmutation-doped silicon production, radiation-effects studies, neutron radiography, and keV neutron beams for tomography and cross-section work.

An improved triple-axis spectrometer and another diffractometer are expected to be built during the next 2 years, and an engineering study has been funded for a possible doubling of the reactor power.

Weapons Neutron Research/Proton Storage Ring Facility (WNR/PSR) Los Alamos National Laboratory

The WNR/PSR being developed at the Los Alamos National Laboratory is a pulsed spallation neutron source for neutron-scattering research in condensed-matter physics, chemistry, materials science, biology, and polymers. It is an interdisciplinary facility that is shared with nuclear- and neutrino-physics research. A beam of 800-MeV protons is provided by the Los Alamos Meson Physics Facility (LAMPF). At present, the WNR can utilize only about 0.5% (~5 μA) of the LAMPF beam. However, the PSR will permit by 1986 the use of 100 μA of LAMPF protons with a much reduced pulse width of 0.27 μsec. At that time, the peak thermal neutron flux in the pulse is expected to be 10^{16} neutrons/cm^2-sec at 12 Hz, making WNR/PSR directly competitive in neutron intensity with the new British pulsed source (SNS) at the Rutherford Laboratory.

At present six beam lines are available for condensed-matter research, three each for elastic and inelastic scattering studies. Two of these instruments, a filter difference spectrometer for vibrational spectroscopy and a single-crystal diffractometer, are operated in a user mode, while the remaining instruments are under development. A general-purpose powder diffractometer is expected to become a user instrument in 1984. A program advisory committee (shared with ANL) currently

meets twice a year to decide on proposals for beam time. The total time available for neutron-scattering studies currently is 60 percent of the LAMPF operating schedule (6 months/year in 1982-1983) and will increase to 80 percent in 1986. A total of ten neutron-scattering instruments is planned for completion by the end of 1986.

Summary of Facilities

Other neutron-diffraction facilities also exist at smaller university reactors for student training and research, most notably several instruments at the University of Rhode Island. In Table 1 we summarize the neutron-scattering instruments currently available at major U.S. neutron sources. The table shows that there are a total of 53 instruments (compared, e.g., with 114 instruments currently operating and over 40 under development in Western Europe). The relative effectiveness of these facilities is, of course, closely related to intensity, energy and momentum range, and flexibility, for example, factors that are impossible to reflect in a single table. In general, current neutron-scattering capabilities in the United States are clearly still competitive internationally in the areas of triple-axis spectrometry with resolutions `0.2 meV, single-crystal and powder diffraction for both steady-state and pulsed sources, polarized-beam research, high-resolution biological diffraction, and neutron interferometry. In a later section, critical neutron instrumentation and measurement capabilities currently unavailable or not fully competitive in the United States will be summarized.

TABLE 1 Summary of Neutron Scattering Instruments Available in the United States

A. RESEARCH REACTORS

1. Diffractometers

	Two-Axis	Two-Axis (Multisector or PSD)	Four-Circle	Four-Circle (PSD)
BNL	-	1	2	1[b]
MIT	2	-	-	-
NBS	-	1[a]	1	1[b]
ORNL	1	1	1	-
MURR	-	2	2	-

2. Spectrometers

	Inter-ferometer	SANS	Three-Axis	Time-of-Flight	Polarized Beam
BNL	-	2[b]	5[c]	-	-
MIT	1	-	-	-	-
NBS	-	1	4[c]	1	-
ORNL	-	3	4	1	2
MURR	1	1	1	-	-

B. PULSED NEUTRON SOURCES

1. Diffractometers (Elastic)

	Powder	Single Crystal	SANS	Beam
ANL	2[a]	1	1	1
LASL	1	1	-	-

2. Time-of-Flight Spectrometers

	Chopper Analyzer	Crystal Analyzer	Filter Crystal
ANL	2	1	-
LASL	-	-	1

[a]Dedicated high-resolution powder diffractometers.
[b]These instruments configured primarily for biological structure research.
[c]One of these three-axis instruments is sometimes used for polarized beam studies.
[d]Primarily for structure of liquids and glasses.

It should also be noted that aside from the facilities described above, there are ongoing state-of-the-art efforts at the various neutron centers in the development of area detectors, multilayer focusing and polarizing monochromators, focusing collimators, neutron interferometers and choppers, all of which are important for the development of advanced instrumentation for reactor or pulsed sources. While in some cases U.S. laboratories have been pioneers in such advances, our efforts in general have a low-to-modest level of support and manpower compared with instrumentation development projects in Europe (some of which are described below). As a result, the implementation of new classes of instruments based on these developments has been generally much slower in the United States.

THE USER COMMUNITY

The U.S. neutron-scattering user community has changed considerably since the 1977 report of the National Research Council (Neutron Research on Condensed Matter, National Academy of Sciences, Washington, D.C., 1977), both in the number of users and in the kinds of science being done. A summary of the total number of users per year at U.S. neutron-scattering facilities during the past 6 years is given in Figure 1. For the purposes of this report a “user” has been defined as a scientist who directly participated in a neutron-scattering experiment at least once during a given year. A scientist who visited a given neutron center more than once to perform experiments is counted only once.

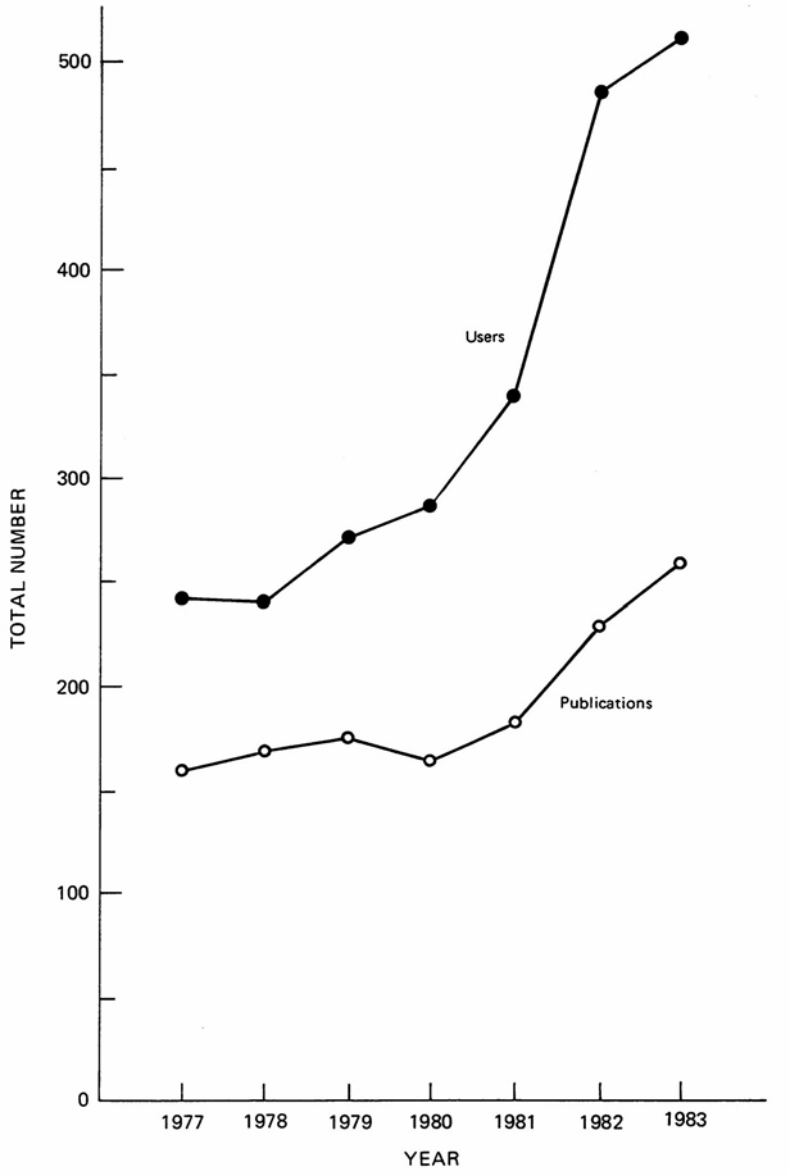

FIGURE 1 U.S. neutron-scattering research--users and publications.

No attempt has been made to identify scientists who might have used more than one neutron source. Also shown in Figure 1 are the number of publications in the 1977-1983 period.

The user trends in Figure 1 show that the number of U.S. users of neutron-scattering facilities has more than doubled during the past 6 years and has gone up 80 percent between 1980 and 1983. This rapid increase in the total user community is broadly reflected in the individual numbers for the majority of the neutron research centers. Major factors include the installation of new or improved small-angle scattering facilities at the research reactors, the commissioning of the Intense Pulsed Neutron Source at Argonne National Laboratory, and other reactor instrumentation developments including high-resolution diffraction and improved polarized-beam and triple-axis spectrometers. It should be noted that this large increase occurred in spite of the shutdown of the CP-5 reactor at Argonne during 1978-1979. It is clear from the user trends that, as has occurred in Europe, the introduction of new or improved neutron instruments that provide new measurement capabilities greatly increases the utilization of such neutron facilities by the scientific community.

The expanded neutron-scattering community shown in Figure 1 also reflects a significant change in the distribution of users from the various scientific disciplines and in some cases the introduction of almost entirely new user groups (e.g., polymer science). In broad terms, the neutron user community in 1983 is distributed as follows: condensed-matter physics, 35 percent; chemistry, 23 percent; materials science, 16 percent; polymer science, 13 percent; biology, 13 percent. Thus while condensed-matter physics has shown

a healthy increase over the past 6 years (~33 percent), these users now represent a considerably smaller percentage of the total community than in 1977 (~45 percent). Other user groups, most notably in polymer and materials science and biology, have shown much greater relative increases (~150 percent), stimulated largely by the availability of new state-of-the-art SANS and high-resolution diffraction facilities. The chemistry community has also grown at approximately twice the rate of the condensed-matter physics community.

Since the number of full-time scientists at the major neutron centers has increased very little during the past few years, these numbers represent a decided increase in part-time users of neutron-scattering facilities. In fact, this has put a great strain on the scientific and technical staff at the National Laboratories in seeking to serve the increasing user community while continuing to meet the program needs of their own agencies. Currently the approximate distribution of users is as follows: federal laboratories and agencies, 30 percent; universities, 60 percent; and industry, 10 percent.

The breadth of the current neutron-scattering community is reflected in the diversity of the organizations that participate in research at the various neutron centers. A list of universities, industries, and laboratories doing independent or cooperative neutron research during this past year is given in Appendix A. One notable trend in the user distribution is the considerable increase over the past 6 years in the number of students using neutron-scattering facilities either full time or part time in their research. Between July 1982 and June 1983, there were 92

student users at the various neutron centers. This number is both significant and encouraging since the education and participation of young scientists in modern neutron-scattering science is essential for the future health and vitality of the field. It should be noted here that, while the majority of users utilize the federal laboratory facilities (almost 90 percent in 1983), the university facilities have trained or provided facilities for close to 30 percent of the student users.

Another measure of the productivity and vitality of the neutron-research community is, or course, the number of publications resulting from the use of neutron-scattering facilities. The publication numbers assembled from the various neutron centers for the past 6 years are shown in Figure 1. It can be seen that a large increase in neutron-scattering publications has occurred that roughly parallels the rapid increase in the user community. Thus we observe an increase of slightly more than 60 percent over this period, almost all during the past 3 years. This increase is smaller than the overall percentage increase in users. This lag is to be expected for new users (in many cases using new facilities) in any field. In fact an even greater lag in publications was noted during the rapid expansion of users at the Institut Laue-Langevin (ILL) in Grenoble during the 1970s. In addition it should be noted that part-time users of any major facility will rarely be as productive in publication as the core of full-time users (who represented a much larger fraction of the total neutron user community in the mid1970s). As will be seen below, the current number of publications per user compares quite favorably with comparable figures for the ILL and other European facilities.

It is also interesting to note that a combination of the facility numbers in Table 1 with the user figures in Figure 1 gives about 10 users/instrument. This is rather close to the comparable ratios assumed for synchrotron facilities in the Report of the Subcommittee on U.S. Synchrotron Radiation Facilities (Current Status of Facilities Dedicated to the Production of Synchrotron Radiation, National Academy Press, Washington, D.C., 1983).

COMPARISON WITH THE EUROPEAN COMMUNITY

We now present a brief review of foreign neutron-scattering users and facilities, concentrating on Western Europe, where the major expansion has occurred during the past 12 years. Western Europe has over the last decade developed a user community more than double the size of that in the United States, driven by a major investment (most notably at the ILL) in new classes of instrumentation and a highly organized, well-funded user policy. A summary of users and publications over the past 6 years is given in Figure 2. In developing the user numbers we have applied the same criteria as we outlined above for the United States, but there is a greater uncertainty in the "user" figures for non-ILL facilities owing to the greater chance of "double counting" scientists who use both ILL and their own neutron facilities. It should be noted that while the total European user community tripled during the 1970s, the period shown in Figure 2 shows a less dramatic rise, reflecting the saturation of facilities at ILL and elsewhere. A notable feature of these current-user

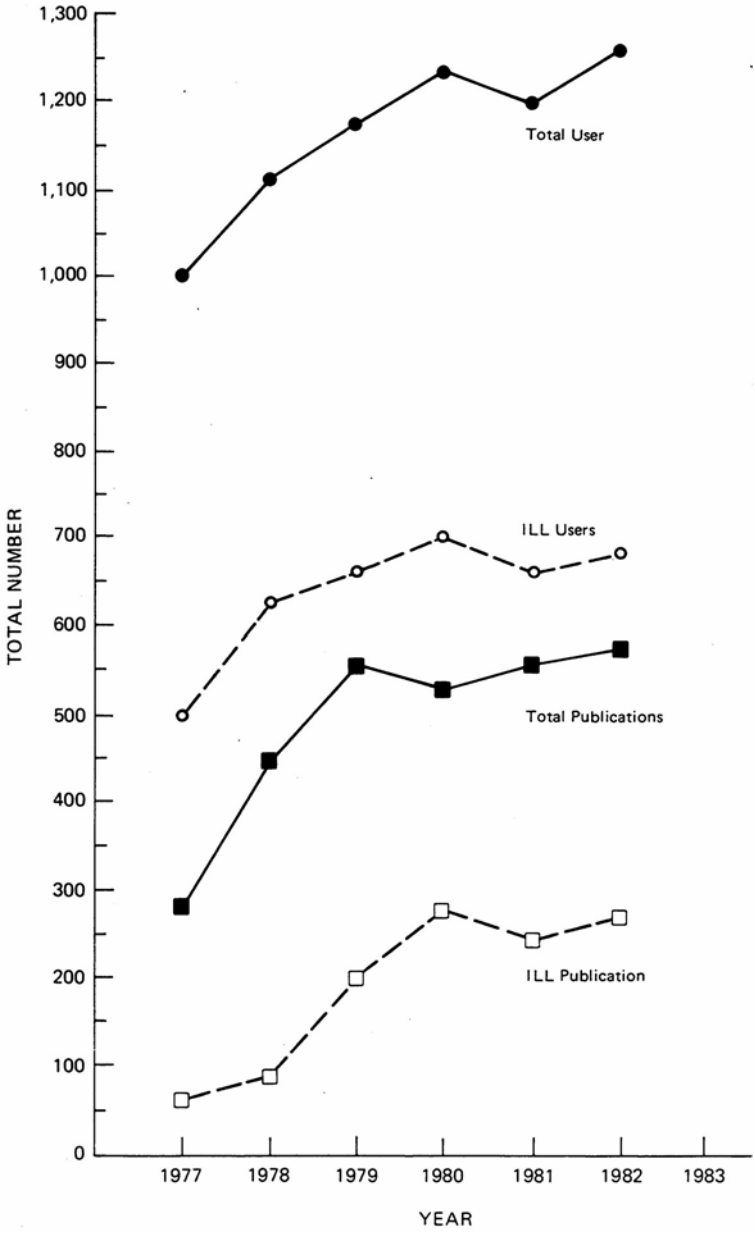

FIGURE 2 Summary of users and publications from Western Europe.

numbers is the dominant position of ILL, which accounts for about half of the users and publications in Western Europe. In fact, the figures show that the ILL alone has about 25 percent more "users" than the total for the United States. The current number of neutron-scattering instruments at the ILL is 26, and the total annual budget (including a program to fund the expenses of users from France, Germany, and Great Britain) is about $25 million (roughly the same as the entire U.S. effort in neutron-scattering research). Taking into account the rapid development and planning of new instruments (~50) in Western Europe, a user community exceeding 1500 would be expected by about 1987.

Beam time on the ILL is scheduled almost entirely in the "user" mode through the review of formal proposals by panels assembled to represent various disciplines and kinds of instruments. In addition, every neutron facility has instrument-responsible scientists and technicians associated with it who are assigned to assist outside scientists in using the facilities. While the average number of users per instrument per year in this mode (about 20) is considerably higher than in the United States, the number for the United States (10) is somewhat higher than the average of the other European facilities. Publication rates per user are roughly the same for the United States as for Western Europe. By comparison, figures for neutron-scattering publications in Canada, which has maintained a traditional role in this field, show an average rate of about 40 publications in recent years. The Japanese, who are engaged in a vigorous expansion in both reactor-based and pulsed neutron research, now show a publication rate approaching 100 papers per year. While these comparisons attest to the continuing productivity

of the U.S. neutron centers, the U.S. ability to serve the needs of the user community is limited by the lack of incremental resources for scientists and technicians to provide direct user support at the major neutron centers.

Another key problem facing the U.S. neutron facilities in seeking to maintain an internationally competitive position in this field is the lack of resources for the development of new classes of instrumentation (leading to new science). A major advantage of the ILL and other European centers over the past decade has been the flexibility and funding to develop such new instruments and the cold neutron sources, guide tubes, and focusing monochromators, for example, needed for their development. In the next chapter we will briefly review the impact of this relative lag in U.S. capabilities.

4.

OVERSEAS NEUTRON-SCATTERING FACILITIES

RESEARCH REACTORS

In this chapter we provide a selective review of foreign neutron-scattering facilities, concentrating on instrumentation developments that have not been matched in the United States. Current activities in the modernization or expansion of facilities in Western Europe and Japan will also be summarized. Again much of our focus with respect to steady-state neutron sources will be on the rapid developments over the past decade at the Institut Laue-Langevin (ILL). It should be recalled, however, that much of the impetus for the European advances was work done at smaller centers, e.g., Jülich, Germany (SANS, backreflection spectrometry), Saclay, France (SANS), Munich (guide tubes). Another key to the European success has been the development and use of cold neutron sources and associated guide halls to create instruments for ultra-high-resolution and high-sensitivity spectroscopy (currently providing energy resolutions as much as 5 orders of magnitude better than available in the United States), small-angle and medium-resolution diffraction, and a variety of other new scientific applications (e.g., ultra-cold neutrons). These sources and related new instrumentation represent the major advances in neutron-scattering capabilities since the mid-1970s, and their development continues to grow in both Europe and Japan. At present, there is only one cold neutron source in the United States (at Brookhaven National Laboratory) and one other is under development (at the National Bureau of Standards). Guide halls to improve the versatility

and flexibility of cold or thermal neutron instruments currently do not exist in the United States. On the other hand, 60 percent of the neutron-scattering instruments at the ILL (16) are located in a large guide hall, and this fraction will rise when a new guide hall and cold source are completed over the next 2 years.

In Table 2 we list the characteristics of neutron instruments at the ILL (mainly brought on-line since the mid-1970s) that either do not exist in the United States or have characteristics of intensity or resolution that significantly surpass comparable instruments in this country. A number of instruments with comparable characteristics also exist (and in fact were developed) at other European centers, e.g., Jülich (Germany), Saclay (Orphèe) France.

The summary in Table 2 does not reflect the entire picture of new capital investment and advanced instrumentation development in Europe. For example, major efforts in the development and construction of focusing monochromators, polarizing devices, reflecting supermirrors, environmental control systems, and dedicated instruments for diffraction surveys using neutron cameras attest to the continuing highly organized efforts to build new and more efficient instruments at steady-state sources in Europe. Moreover, currently under development at the ILL is an improved D_2 cold source and a second D_2 cold source that will serve six new instruments to be installed in a new guide hall by 1985. Further, there is a new reactor center (Orphèe) at Saclay near Paris with two H_2 cold sources that will ultimately commission 20 new instruments for neutron-scattering and fundamental physics research. An expanded guide hall with 9 new instruments

TABLE 2 Unique Scattering Facilities at the Institut Laue-Langevin[a]

Instrument	Location	Wavelength/Energy/Wave-Vector Range	Areas of Application
IN-5 Multichopper spectrometer	Cold guide	10 μeV-30 meV/0-2.3 $Å^{-1}$	Low-energy excitation and quasi-elastic scattering in all materials
IN-6 Focusing time-of-flight spectrometer	Cold guide	70 μeV-30 meV/0-2.6 $Å^{-1}$	Quasi-elastic scattering and low-energy density of states for chemical and biological materials, catalysts, low-dimensional systems etc. (very high sensitivity)
IN-10 Backreflection spectrometer	Cold guide	0.3 μeV-100 μeV/0-2.6 $Å^{-1}$	Low-energy excitations (phonons, tunneling states, etc.) and diffusive process in solids and liquids
IN-11 Spin-echo spectrometer	Cold guide	25 neV-1 meV/0.02-2 $Å^{-1}$	Ultra-high-resolution spectroscopy of relaxation processes in polymers, biological matter, spin glasses, ferrofluids, etc.
IN-13 Backreflection spectrometer	Thermal guide	8 μeV-1 meV/0-6 $Å^{-1}$	Low-frequency dynamics, phase transitions, tunneling processes, diffusion in chemical materials, hydrogen in metals, polymers, etc.
D-5 Three-axis spectrometer with polarization analysis	Hot source	0.4-1.1 Å/50-400 meV	Polymerization analysis of magnetic-system studies of resonant nuclei possible
D-7 Diffuse-scattering spectrometer	Cold guide	$\geq$100 μeV/0-2.6 $Å^{-1}$ polarization analysis	Static and dynamic aspects of short-range order in materials, paramagnetic scattering; uses polarized neutrons
D-9 Low-wavelength four-circle diffractometer	Hot source	0.4-0.8 Å	High-precision, medium-resolution studies of electron density, thermal parameters, and atomic disorder
D-11 Small-angle scattering instrument	Cold guide	5-20 Å/5 x 10^{-4}-0.3 $Å^{-1}$	The world's best neutron instrument for studying polymers and biological assemblages, microstructure, defects, pores in materials, magnetic clustering, etc.; exceeds state-of-the-art U.S. instruments in intensity and wave-vector range

wave-vector four-circle diffractometer			membranes, surface slider
D-17 Low-angle diffractometer	Cold guide	4-10 Å/0.005-0.5 Å` 1	SANS and medium-resolution diffraction on macromolecules and biological systems
D-20 Two-axis diffractometer with curved PSD	Thermal beam	1-3 Å/0-7 Å` 1	High-sensitivity, rapid-powder, liquid and glass diffraction, real-time structure studies
IN 1B Hot source three-axis spectrometer	Hot-source beam	0.4-1.5 Å/30-400 meV	High-energy excitations in molecular solids, magnetic materials, metal hydrides, etc.
IN 14 Wide-range cold-neutron triple axis	Cold guide	0-15 meV/0-4 Å` 1	Dynamics of structural phase transitions, critical scattering, etc.
IN 15 High-resolution spin-echo spectrometer[b]	Cold guide	` neV/0.01-0.3 Å	Dynamics of macromolecular systems
DB 21 Dedicated small-angle diffractometer for biologyb	Cold guide	5-10 Å/0-1 Å` 1	High-sensitivity, low-resolution studies of large biological structures (~0.5-mm crystal sizes)
Ultra-high-resolution diffractometer	Cold guide	4-10 Å/0-3 Å` 1	Crystallography of materials with large volume unit cells

[a]Instruments that either do not exist in the United States or whose characteristics are not fully matched in this country. In may cases, analogous instruments exist or are being developed at other European centers, e.g., Orphèe, Jülich, Riso.

[b]Under development at new cold source.

is also under construction at the KFA Research Reactor in Jülich. Finally, the Japanese government has approved funding for the complete modernization of the JAERI III reactor at a cost of ~$150 million, including a replacement of the vessel, an upgraded fuel and beam-tube arrangement, and installation of a large cold source and guide hall.

The total current operating expenditures for neutron scattering at research reactors in Western Europe is about $80 million/year (in fiscal year 1983 dollars) including associated reactor operation costs, roughly triple the U.S. effort. An order-of-magnitude difference emerges when one compares capital investment for new spectrometer development and construction efforts. Aside from recent new reactor construction (Saclay) and modification (Berlin), currently ~$45 million worth of new or advanced neutron-scattering instruments and guide halls are either being commissioned or under development, primarily in France and West Germany but also in Sweden and Denmark. There is also a proposal for a major redevelopment of the Munich university research reactor to provide a new advanced center for neutron-scattering research.

The consequences of this investment gap over the past decade between European and U.S. research reactors is being increasingly felt in our inability to compete in many areas of new science related to high-resolution neutron spectroscopy, small- and medium-angle diffraction, and diffuse scattering, for example. Further, the high degree of flexibility and efficiency afforded by the development of cold sources, guide-tube technology, and beam-focusing techniques has not been pursued in the United States. Fortunately, the major U.S. research reactors are still world class in terms

of available thermal-neutron-beam intensities, and there are immediate opportunities to achieve a competitive status in advanced instrumentation for both cold and thermal neutron scattering, which will be outlined in Chapter 6.

PULSED NEUTRON SOURCES

The current U.S. position in pulsed neutron research and development is better in relative terms with respect to foreign competitors than is the case for steady-state sources. For example, the intense pulsed neutron source at Argonne National Laboratory is, for the present, the highest-intensity facility in the world, and the WNR/PSR is scheduled to provide by 1987 an order-of-magnitude increase in intensity for pulsed-neutron experiments. However, developments abroad make current comparisons highly misleading. For example, the SNS advanced spallation source under construction at the Rutherford Laboratory is scheduled to be brought on line by the end of 1984, with neutron intensities 2-3 times the current IPNS performance and will ultimately (by 1986) generate a current of 200 μA of 800-MeV protons on a spallation target, thus providing a peak thermal flux of 5×10^{15} neutrons/cm^2-sec at a 50-Hz repetition rate, roughly twice the total intensity of the scheduled WNR/PSR source. This facility will ultimately have a complement of at least 15 neutron-scattering instruments, providing unmatched flexibility. Moreover, the Japanese, who have developed a modest-flux facility at Tsukuba with an impressive array of instruments, are also funding a planning and design study for a major new pulsed source (cost ~$100 million in fiscal year 1983

dollars) that would slightly exceed the characteristics of the SNS.

Perhaps of greatest potential impact on the long-term development of pulsed neutron sources, is the extensive study and design effort under way at the KFA in Jülich, West Germany. This major planning project with a budget of ~$6 million/year is aimed at the possible ultimate construction of a pulsed spallation source with an ~10^{17} neutrons/cm^2-sec peak flux and a time-averaged flux exceeding 10^{14} neutrons/cm^2-sec. The potential cost of this facility (~$300 million to $400 million capital, ~$30 million/year operating) of course raises large scientific and political questions in the European community and will, at the very least, require a broad multidisciplinary base of support. The development of a source with these flux characteristics is perceived necessary by the German group in order to match or surpass the capabilities of modern high-flux reactors for low-energy neutron research and at the same time to exploit fully the new opportunities offered by pulsed sources, particularly for high-energy (>100-meV) neutron scattering. The study also includes a major effort to develop concepts and designs for a new generation of scattering instruments. Active efforts in new instrument designs are also a major part of ongoing activities at the Rutherford Laboratories in Great Britain, in Japan, and at the Argonne National Laboratory (ANL) and the Los Alamos National Laboratory (LANL) pulsed sources. The two U.S. pulsed neutron efforts currently have a combined budget for source operations and

scientific costs of about $10 million/year.[2] While this amounts to about 40 percent of the total U.S. neutron-scattering funding, it still does not, for example, allow full-time operation of the IPNS source. In addition, this funding level provides only marginal discretionary resources for the development of new instrument or source concepts. Again, as for U.S. research reactors, there are important opportunities for future pulsed-source development and research activities, which will be outlined in a later section.

[2]This figure assumes $2 million as the share of scientific and facility operating expenses provided at the WNR by the Office of Military Applications (OMA) of Department of Energy and discretionary LANL funds. The apportionment of funds provided by OMA for the development and scientific use of the WNR/PSR between nuclear or weapons-related research and materials-science applications is a complicating factor in the exact assessment of current neutron-scattering research funding but does not substantially affect the comparisons of U.S. and Western European funding included in this report.

5.

RECENT NEUTRON-SCATTERING RESEARCH IN THE UNITED STATES; COMPARISONS WITH EUROPE

In this chapter we present selected summaries of important research areas and accomplishments during the past 6 years. These summaries have been coordinated by experts on the panel in the appropriate scientific disciplines involved and reviewed by the panel as a whole. The focus is generally on U.S. neutron-scattering work, except in cases where activity has been dominated by special capabilities abroad (e.g., high-resolution spectroscopy, broad areas of polymer and chemical research). Where the work involves new areas of scientific applications of neutrons that have evolved recently (e.g., polymer and materials science, biology, chemical spectroscopy), we have tried to provide more background to explain the special role of neutrons in these cases. An attempt has also been made to point out both new directions in science and examples of broad areas where instrumentation at U.S. neutron sources does not allow critical scientific opportunities to be pursued.

CONDENSED-MATTER PHYSICS

Physicists were the first scientists to exploit the unique properties of the neutron in studying condensed matter, and after 30 years of intense activity the level of interest and vitality of the field are undiminished. In the following

paragraphs we survey the contributions that neutron scattering has made to the various subfields.

It is worth reflecting that most of the results discussed represent not only significant advances in our understanding of the physics of the materials but that neutron scattering provided unique information not available from other known techniques. Two examples, discussed more fully in subsequent sections, illustrate this particularly well. The first is the development of magnetic order in superconductors, where a series of key discoveries beginning in the late 1970s and involving a close interplay between imaginative materials synthesis and neutron-scattering studies have caused the simple dictum that "superconductivity and magnetism don't mix" to be greatly revised. In this case although thermodynamic and magnetic measurements suggested the occurrence of unusual phenomena in those new materials, neutron scattering was essential to establish its nature.

A second example is provided by ongoing recent studies of the effect of disorder on the collective behavior of condensed-matter systems. Major conceptual difficulties have arisen in recent years as to the behavior of a simple magnetic model system when placed in a magnetic field that varies randomly in direction from site to site. Although the model has attracted much interest as a prototype of real physical disorder, the production of such a random field on an atomic scale is experimentally not possible. However, as it turns out, the application of a uniform magnetic field to a dilute random antiferromagnet produces a random antiferromagnetic internal field and a physical situation that simulates the ideal theoretical model. Neutron-scattering measurements on such systems are now providing the critical

experimental tests of our understanding of simple random systems.

Magnetic Systems

The determination of magnetic structures was one of the first and most important applications of neutron diffraction. While many of the interesting magnetic structures of simple materials have now been determined, the ability to make these determinations on new materials will be essential for the indefinite future as long as new materials are developed. Most magnetic structures have been determined at medium-to low-flux sources using a two-axis diffractometer, but for very complex structures (Nd, PrAg, TmS), or for fine structural details (MnP), the polarization analysis technique can be extremely valuable. Use of this technique has been limited because there are only a few spectrometers in the world equipped for these measurements.

Amorphous ferromagnets have enormous potential value in commercial applications, and neutron scattering has been used in a variety of ways to understand these materials on a microscopic basis. Diffuse scattering measurements have been used to obtain the radial distribution functions that describe the basic structure, inelastic neutron-scattering studies have given details of the spin dynamics, and small-angle scattering has been used to study the microstructure. Neutron experiments on these materials have been carried out worldwide. The advantage of using polarized neutrons has not yet been fully exploited in these studies. Another class of materials that has attracted great experimental and theoretical interest in recent years is that group of

rare-earth materials in which the rare-earth ion apparently has a fractional valence--the intermediate- or mixed-valence materials. These materials do not show magnetic order, and the neutron-scattering spectra show a broad quasi-elastic line with an energy width in the range from 10 to 100 meV. The shape of this line is consistent with a fast (10^{-13} sec) relaxation process of the rare-earth spins. Actinides frequently show many characteristics of the unstable 4f moment systems. In the rock salt uranium compounds, for example, experiments have shown that, even though the systems order magnetically, spin waves need not exist. A combination of x-ray photoemission spectroscopy (XPS) and neutron spectroscopy suggests that the unusual damping is caused by strong 5f-6d electron interactions. Both critical and inelastic magnetic scattering has contributed greatly to our understanding of the solid-state physics of the last row of the periodic table. In another kind of experiment, polarized neutrons have been used to measure the induced magnetic form factor in order to gain a better understanding of the behavior of the f electrons in these materials. In general, these form factors are not dramatically different from free-ion form factors for integral valence ions. Interesting exceptions are CeSn and CePd, where evidence of some 5d polarization is found at low temperatures.

As an example of the subtlety of magnetic systems and of the continuing long-term need for state-of-the-art neutron-scattering facilities, it should be noted that new and exciting facts about the most studied of all magnetic materials, Cr, Fe,and Ni, are still being discovered through neutron-scattering experiments. Recent polarization analysis experiments of the diffuse scattering from Fe and Ni in the paramagnetic

phase have revealed short-range magnetic order extending well above T_c. In another type of polarized-beam experiment, the appearance of "forbidden" magnons in Ni well below T_c indicates a deviation in the local and bulk magnetization directions. Commensurate diffuse excitations have been observed in the incommensurate spin-density wave state of Cr metal. These excitations were completely unexpected and are not yet understood. All of these experiments give valuable insights into the fundamental nature of the magnetic behavior of these important metals.

Practically all areas of magnetic research would benefit from more and improved neutron polarization analysis spectrometers. Higher source fluxes and improved polarizers are both important for the growth of this technique. Fortunately, recent advances in this country and Europe toward better polarizers have been made. Pulsed-neutron sources show promise for enabling inelastic magnetic scattering at high-energy transfers. For example, recent measurements have already extended the spin-wave spectrum in Fe to higher values than previously possible, and such sources promise new opportunities to locate the single-particle (Stoner) continuum. The lack of very-high-resolution instruments, such as a neutron-spin-echo spectrometer, has limited the U.S. research in important areas, such as the relaxation effects in spin glasses.

Phase Transition

From its inception, neutron scattering has made important contributions to the field of phase transitions and critical phenomena. Not surprisingly, this has continued to be the

case for the past 6 years. Phase transitions occur in a wide variety of systems so that the work discussed in this section will overlap with results presented in most of the other sections. There has been an interesting evolution in the class of materials and the types of problems being pursued. Initial work, especially in the period 1965 to 1975, concentrated on prototypical phase transitions in model systems. Examples include soft modes in ferroelectrics and in other systems exhibiting structural transitions such as $SrTiO_3$, ordering in binary alloys such as CuZn, and magnetic transitions in simple magnets such as $RbMnF_3$, K_2NiF_4, Fe, and Ni. These experiments were invaluable in elucidating the basic principles governing critical phenomena.

As a result of these early studies and of important advances in theoretical understanding, it has proven possible to address much more complicated issues. Recent neutron work has concentrated on the phase-transition behavior of more exotic systems. Indeed a number of the more interesting experiments involve issues that were barely conceived of at the time of the previous NAS report. Examples include random field effects, spin-Peierls transitions, devil's staircase phenomena in incommensurate systems, re-entrant superconductivity, re-entrant spin-glass behavior, and other effects originating from competing interactions. In each case neutron-scattering experiments have provided a key to understanding the basic physics underlying these phase transitions. It is also interesting to note that with a few important exceptions, the crucial experiments have involved conventional elastic and inelastic neutron-scattering (including SANS) techniques. The most serious limitation typically has been sample size or, equivalently, neutron flux. In

many cases major improvements in momentum or energy resolution, or both, currently available or under development in Europe, will be of increasing importance. In this brief report, it is impossible to survey all the beautiful experiments that have been performed in the last 6 years. We therefore limit ourselves to a few representative samples.

The effects of randomness, especially in systems with competing interactions, are now being extensively explored. Particularly dramatic effects are observed in spin systems with random magnetic fields, that is, magnetic fields with zero average value but nonzero variance. Neutron experiments in both the United States and Europe have verified that a uniform field applied to a random antiferromagnet generates a random staggered magnetic field; this makes possible a systematic study of the phenomena. High-resolution experiments on both two- and three-dimensional systems have revealed that long-range magnetic order is not attained in the presence of a weak random field and that instead one sees with decreasing temperature a continuous evolution from the paramagnetic state to a frozen microdomain state. Such random field effects are undoubtedly important in a range of other physical systems, including random-anisotropy rare-earth amorphous alloys.

Spin glasses have been the subject of intense experimental and theoretical study in recent years, and neutron techniques have contributed greatly to our understanding of these materials. In Europe, a combination of the neutron-spin-echo and polarization-analysis techniques have been used to measure the time-dependent spin-correlation function of Cu-Mn alloys over a time range from 10^{-12} to 10^{-9} sec. In the United States, elastic polarization analysis measurements on single

crystals of Cu-Mn have demonstrated strong short-range magnetic correlations associated with short-range nuclear order. Exotic effects are also observed in alloys with competing ferromagnetic and antiferromagnetic interactions. With increasing concentration of antiferromagnetic bonds one observes an evolution from ferromagnetism to spin-glass behavior. For ferromagnets with concentrations near the crossover point one sees "re-entrant behavior," that is, with decreasing temperature the system evolves from a paramagnet to a ferromagnet to a spin glass. The spin-wave frequency appears to soften at both the paramagnetic-ferromagnetic and ferromagnetic-spin glass transitions. In addition, unusual diffuse scattering is observed in the re-entrant phase, presumably originating from residual microdomains of the ferromagnetic network. These effects have been seen in such systems as Fe_xCr_{1-x}, Fe_xNi_{1-x}, PbA1, and FeMnPC. This is still an active and rather controversial area of research. It should be noted that the most precise experiments have been performed at Grenoble utilizing the small-angle scattering and high-energy resolution spectrometers. Systems with competing anisotropies rather than competing interactions have also been studied. Here again one observes new magnetic states whose basic structures and excitations could only be elucidated with neutrons.

The study of phase transformations and other highly cooperative phenomena is perhaps the most challenging and subtle that condensed-matter physics has to offer. At the same time, fresh ways of thinking about such systems have greatly expanded our ability to understand such systems and suggested subjects for new studies. Such systems are very often magnetic because of their relative freedom from

complicating extraneous interactions. As in the past, neutrons will continue to provide an indispensible tool for such studies.

New Materials and Phenomena

The unique capabilities of neutron studies are readily apparent in the study of the coexistence of magnetic and superconducting long-range order, which was discovered ("engineered" is a better term) in the late 1970s. The phenomenon of superconductivity is quite tolerant of large concentrations of impurity atoms, so long as they are not magnetic in character, but is quickly destroyed by small concentrations of magnetic impurities. This peculiar fact was readily explained by the Bardeen, Cooper, and Schrieffer (BCS) theory, which showed how superconductivity can arise from a binding of pairs of electrons that travel in time-reversed orbits. Magnetic impurities that do not respect time-reversal symmetry destroy the pairing, whereas chemical impurities simply scatter the electrons into new time-reversed orbits leaving the superconductivity intact. The early studies of the magnetic suppression of superconductivity were carried out on simple binary alloys in which magnetic impurity atoms were substituted randomly into the lattice of the superconducting metal. Reasoning that a more stringent test of coexistence would result if the electrons responsible for the superconductivity could be effectively separated from those electrons responsible for the magnetism, new studies were undertaken on more complex ternary systems, in which the magnetic atoms are separated from the atoms responsible

for the superconductivity by a barrier of inert atoms, preventing strong interaction between the two.

In the case of materials such as $DyMo_6S_8$, heat-capacity measurements showed the presence of a new kind of ordering occurring below the temperature of the onset of superconductivity. Neutron-diffraction studies were necessary to establish the nature of the ordering, which was found to be simple antiferromagnetism in which planes of atoms with magnetic moments up and down alternate. The superconductivity is not destroyed, proving that superconductivity and antiferromagnetism can simultaneously coexist at the same temperature. In materials such as $ErRh_4B_4$, neutron-scattering studies have shown that ferromagnetic arrangement of magnetic moments arises at temperatures below that at which the sample becomes superconducting and that in the process the sample regains its normal conductivity. Thus, superconductivity and ferromagnetism can exist in the same material but apparently cannot coexist at the same temperature. Further insight into the nature of the competition between magnetism and superconductivity has recently come from studies of smallangle neutron scattering, which reveal that even when the ferromagnetic state is marginally unstable, an entirely new type of order, taking the form of a long-wavelength oscillating magnetic disturbance can coexist with the superconducting state. These findings may have far-reaching implications for the directions of future research in superconductivity.

Graphite is a prime example of a layered structure composed, in this case, of covalently bound sheets of carbon atoms with adjacent sheets held together more loosely by van der Waals forces. New compounds with unusual properties

can be prepared by inserting, for example, alkali metal atoms between the graphite sheets. Among the fascinating and incompletely understood aspects of these resulting graphite intercalation compounds (GIC) is the structure of the inserted atoms. Neutron-scattering studies have elucidated the nature of the stacking of adjacent metal layers and have shown that at high temperatures the ordering is liquidlike. Unsaturated materials, prepared with low-metal-vapor pressure, have metal atoms inserted between every nth graphite layer, where n is a simple integer. This phenomenon is known as staging. Recent neutron-scattering experiments under hydrostatic pressure have revealed a new fractional staging sequence, related to the n = 3 stage by particle-hole symmetry, whose existence helps to decide between competing theories of the staging phenomenon. A recent first study of the dynamic structure factor and diffusion processes in higher-stage metal-graphite compounds has only been possible by joint U.S.-ILL experiments using high-intensity and high-resolution spectrometers at the ILL.

Models of one-dimensional (1-D) magnetic systems show in addition to linear spin-wave excitations, localized large-amplitude excitations that preserve their integrity as they move along a chain. It is expected that these excitations, called solitons, exist in real materials, and considerable effort has been made to observe them by neutron scattering. Both planar 1-D ferromagnets and antiferromagnets in external magnetic fields are expected to have soliton excitations, although the effects are more difficult to interpret in the ferromagnetic case, where neutron measurements in CsNiF are still controversial. Soliton effects have been successfully observed in the nearly classical S = 5/2 antiferromagnet,

TMMC, by a group at ILL. In $CsCoC1_3$ (S = 1/2), which is an easy-axis antiferromagnet, soliton effects are expected even in the absence of an external magnetic field, and they have been seen by neutron scattering. The longitudinal excitations can be thought of as Doppler-shifted quasi-elastic scattering from moving domain walls (solitons), whereas the transverse excitations involve the creation of domain wall pairs.

A new class of materials that has attracted considerable interest in the past few years are incommensurate systems, in which two subsystems with mutually incompatible translational symmetry coexist. For example, if the instabilities associated with structural phase transformations involve competition between forces of various ranges, the resulting distortion waves may be incommensurate with the underlying lattice. This mechanism was first identified with charge-density wave (CDW) formation in metals, and there have been several recent studies of CDW transformations in quasi-1-D metals such as potassium cyanoplatinate (KCP) and TTF-TCNQ. A related transition, known as a spin-Peierls transition, may occur in S = 1/2 magnetic chains. The transition, which is predicted to be a simple dimerization for nearest-neighbor interactions, has in fact been observed in two different quasi-1-D magnets. Incommensurate phase transformations have also been discovered in insulators, a particularly clean example being potassium selenate (K_2SeO_4), where a low-frequency phonon with an incommensurate wave vector has been observed by neutron studies above the critical temperature. Elementary theory shows that this system has a two-component order parameter and should have critical properties identical to the XY ferromagnet. This has been

verified, in part, with neutron studies. The phenomenon of "locking in," whereby an initially incommensurate lattice distortion becomes pinned at a commensurate value was first observed by neutron studies, and recently an example of electric-field-induced lock-in transformation has been found in the ferroelectric thiourea.

Crystal Dynamics

The frequencies and displacement patterns of the vibrational modes provide the most direct available insight concerning the strength and range of interatomic forces in solids. Optical and electron tunneling spectroscopies provide valuable but limited information concerning vibrational properties. Inelastic neutron scattering has proven the most reliable and complete tool for investigating phonon dispersion relations in solids. The techniques, using triple-axis spectrometers at moderately high-flux reactors are by now classical. They will continue to fulfill a vital need so long as the understanding of the forces in increasingly sophisticated new materials challenge condensed-matter scientists. The interatomic forces in metals are profoundly modified by screening from the conduction electrons. In the case of d-electron metals these screening effects can be seen as more or less sharp anomalous features in the phonon dispersion and provide exacting tests of state-of-the-art electronic-band-structure calculations. Such tests have been provided in recent years through detailed neutron-scattering studies of various transition metals, alloys, and transition metal carbides. Metals with flat or otherwise well-nested portions of Fermi surface can show giant Kohn anomalies, which are

precursors of charge-density wave instabilities such as the Peierls transformation discussed above. Of the various quasi one- and two-dimensional systems studied extensively with neutrons, the 1-D metal (KCP) is the most spectacular. Phonon linewidth effects are a potential rich aspect of e-p interaction largely unexplored with neutrons owing to. lack of energy resolution. Ideas for high-resolution momentum focusing instruments exist but would require higher-flux sources to achieve their full potential.

The presence of a weakly coupled incommensurate chargeor mass-density wave in an otherwise periodic structure gives rise to new gapless excitations, which correspond to relative translations of the density wave. Such modes, sometimes called phasons, differ from true acoustic modes, not only in the nature of the atomic displacements involved but also in the fact that they become overdamped as their wave vector goes to zero, making them difficult to study with optical probes. Such modes have now been seen in several incommensurate systems. In one of these, Hg_xAsF_6, incommensurate mercury chains behave independently at high temperatures, and neutron studies show that at short wavelengths the dynamics are those of a 1-D harmonic fluid. Inelastic neutron-scattering studies have measured the dispersion of longitudinal elastic waves in graphite intercalated with various donor and acceptor atoms. These measured dispersion curves provide direct information on the magnitude and range of the interlayer forces. For example, the graphite-alkali atom coupling is greater than the normal graphite-graphite coupling in pristine graphite, whereas the reverse is true for the acceptor intercalant, $FeCl_3$. Results also scale according to the intercalant areal density, suggesting that every intercalant

atom, but not every graphite atom, contributes to the interplanar stiffness. Although of great interest, from the viewpoint of 2-D physics, it has proven difficult to carry out similarly detailed studies of phonons propagating within the intercalant layers, because of sample size restrictions. This is one example of a limitation imposed by present reactor fluxes.

Defect Systems

To characterize completely the dynamics of hydrogen dissolved in metals requires measurements over a wide range of energy transfer. The diffusive motions result in quasi-elastic scattering, requiring instruments with energy resolution down to 1 μeV. This field of research has been active in Europe using the very high resolution available with neutron backscattering spectrometers. The low-energy vibrational aspects are coupled to the acoustic phonons of the host lattice and have been studied throughout the world using triple-axis spectrometers. The optic modes, or localized modes for dilute hydrides, have been measured by both triple-axis and time-of-flight techniques. The Japanese have demonstrated the value of a pulsed neutron source by measuring local vibrational spectra up to 800 meV. The large incoherent cross section of H makes it possible to perform scattering measurements on dilute solutions, and recent efforts in the United States have extended these spectroscopic studies to samples in the ~0.1 percent H regime where hydrogen embrittlement occurs. These improvements have also provided unique information on the local environment and bonding potentials of hydrogen trapped by impurities in metals. The study of diffusive motions is also important in fast

ion conductors. Here the time scale is somewhat shorter than is the case for hydrogen in metals so that triple-axis spectrometers can be employed. Such experiments have been performed both in the United States (on LiA1, for example), and in Europe (on $SrC1_2$, for example).

The introduction of complex defects with internal degrees of freedom into a crystal lattice produces a variety of interesting effects. Resonant hybridization of the defect states and phonon modes of matching symmetry and energy have been clearly observed in neutron-scattering measurements of dilute $CN^{`}$ impurities in KC1. In the mixed-crystal system $(KCN)_x(KBr)_{1-x}$, the $CN^{`}$ ions freeze into a random distribution of orientations as the temperature is lowered, producing an orientational glass state analogous to spin glasses. This state was discovered through the observation of diffuse elastic neutron scattering.

The greatest shortcoming of the U.S. efforts in the study of defect systems is the lack of very-high-resolution spectrometers for studying quasi-elastic scattering and tunneling phenomena. The backscattering instruments in Europe have given them unchallenged leadership in such fields as hydrogen diffusion.

Surfaces and Overlayers

At the time of the NAS report on Neutron Research on Condensed Matter in 1977, a few demonstration neutron experiments on surface phenomena had been reported. As we shall discuss in this section, this has now developed into a major area of research with active programs at many major facilities in the United States and Western Europe. It seems clear

that this field will continue to grow, and, indeed, certain of the problems (e.g., high-energy spectroscopy) are well matched to pulsed neutron sources, so that one can expect major activity at the new pulsed sources as they come online. Because neutron source intensities are relatively low, and further since neutrons interact weakly with matter, one might expect that surface signals would be undetectably low. This is indeed the case for virtually all single-crystal surface experiments. However, there is a variety of microcrystalline substrates, most notably exfoliated graphite, with surface areas as large as 40 $m^2 g^{-1}$. Thus for a 2.5-cm^3 sample the illuminated surface area may be as large as 300m^2. In favorable cases, it is then possible to separate out scattering events that originate from physisorbed or chemisorbed overlayers from the bulk scattering. Elastic, quasi-elastic, and inelastic neutron-scattering studies of surface overlayers have now all been reported. The most detailed studies to date have been for rare-gas atoms, diatomic molecules, and hydrocarbons physisorbed on graphite. Some experiments in thick films and on co-existing bulk and film phases have also been reported. They involve primarily powder diffraction with an energy analyzer to eliminate inelastic events or else inelastic scattering using triple-axis or time-of-flight techniques. In most cases, the essential limitation has been absolute signal levels. Thus, an increase in neutron flux by an order of magnitude would have a fundamental impact on this field.

Elastic-scattering experiments yield information on the overlayer structures and transitions. The first such studies were on atoms and diatomic molecules physisorbed on graphite; species studied with neutrons include H_2, D_2,

^{4}He, ^{3}He, Ar, and N_2 on graphite. All of these exhibit triangular structures with a lattice constant either commensurate or incommensurate with respect to the graphite substrate. By changing the coverage, the temperature, or both, it has been possible to study both commensurate-incommensurate and melting transitions. The structures of the various phases have been accurately determined, but because of flux limitations, only qualitative information has been obtained on the details of the phase transitions.

Systems exhibiting more complicated phases and phase transitions have also been studied with elastic neutron-diffraction techniques. These include O_2, CF_4, N_2, C_2D_6 (ethane), and C_5D_{12} (butane) on graphite as well as C_5D_{12} (neopentane) on TiO_2. Bilayers of O_2 on graphite exhibit an antiferromagnetic transition at 12 K, and evidence for the concomitant superlattice peak has been obtained. For nonspherical molecules the structures may be quite complicated; the unit cell may be a low-symmetry parallelogram, and the molecules may be tilted with respect to the surface. Such structures have been solved for butane and N_2O_2 on graphite. The butane system also appears to exhibit quite interesting melting behavior. Very recently, diffraction studies have been reported for CD_4 and Ar on $NiC1_4$. It has also been realized that these physisorbed systems may exhibit co-existing bulk and film phases with reversible transitions between the surface and bulk structures. Such effects have now been seen directly with neutrons for C_2D_4 on graphite.

Of course, one of the salient advantages of neutrons over other scattering techniques is the ability to study dynamics in the range of typically 0.1 to 100 meV. So far, only a limited number of inelastic-scattering experiments

have been carried out on surface systems. Interesting results have been obtained in both the United States and Europe for hydrogen chemisorbed on metallic surfaces such as Raney Ni, platinum, and palladium blacks. These are all of fundamental interest in the field of catalysis; vibrational excitations are observed whose frequencies match well to the results of model calculations. Collective effects have also been studied using triple-axis techniques. For example, the phonon density of states for monolayer argon on graphite has been obtained; the in-plane results can be reasonably well described at low temperatures by a two-dimensional roton. Finally, a limited number of quasi-elastic experiments probing surface diffusion have been performed. Particularly interesting behavior has been observed for CH_4 on graphite near melting.

Clearly, this is a vigorous, rapidly expanding field in neutron scattering. We expect that an increasing number of experiments will be performed on high-surface-area substrates, especially those relevant to catalysis. Increased flux would greatly facilitate these studies.

Liquids and Glasses

Neutron-scattering techniques have provided the most detailed and complete experimental results on the structure and dynamics of isotropic systems in both the liquid and amorphous states. These systems present one of the outstanding challenges in statistical physics, since, in contrast to solids, there is no available first-order theory in terms of independent quasi-particles such as magnons and phonons. Indeed, progress has only been possibly by detailed comparison of the results

of neutron scattering with the results of molecular-dynamics simulations, a technique that has so far been more successful for liquids than for glasses or amorphous solids. Nevertheless, real progress has been made in recent years in a fundamental understanding of the statistical physics of these systems, particularly in the use of kinetic theories. An area in which the above considerations do not apply is that of the quantum fluids ^{3}He and ^{4}He, where neutron scattering has been used to study the detailed predictions of available theories. In the following, we describe some examples of results over the past 6 years that illustrate the power of the technique and the progress being made.

Quantum Fluids

Recent neutron inelastic scattering studies have revealed the elementary excitation spectrum of ^{3}He for the first time, stimulating intense theoretical effort and greatly increased understanding of the underlying physics of Fermi liquids. In view of the extremely high neutron absorption cross section of ^{3}He, these experiments represent an unrivaled tour de force of experimental techniques. Future research in this area will provide new insights into the dynamics and quasi-particle excitations in ^{3}He, ^{4}He, and mixtures of the two isotopes, leading to new theoretical advances in the understanding of quantum liquids. These studies will be greatly enhanced by the availability of intense beams of epithermal neutrons from pulsed spallation sources.

An outstanding problem in quantum statistical mechanics has been the existence and properties of a Bose condensate in superfluid ^{4}He and the nature of the momentum distribution

in both normal and superfluid He. Recent neutron-diffraction results have led to very precise estimates of the condensate fraction in superfluid ^{4}He, while high momentum transfer experiments on normal and superfluid ^{4}He using epithermal neutrons show promise of giving very detailed measurements of the momentum density distribution, but again increased fluxes are needed to provide the necessary resolution and sensitivity.

Classical Liquids

One of the outstanding results from neutron-scattering studies of classical liquids in recent years has been the measurement of the density dependence of both the static and dynamic structure factors in dense krypton gas. These results give direct information about the nature and magnitude of the three-particle correlations in this system for comparison with the predictions of statistical physics, and thus promise much better models for these many-body effects. Additional progress can be expected as higher-intensity time-of-flight instruments and pulsed sources become available for measurements of the structure and dynamics of simple fluids.

Recent results from neutron-scattering studies of liquid crystals at reactors in Europe have identified the existence of hydrodynamic instabilities and time-dependent states and phase diagrams with multicritical properties in liquid crystals. Further progress in this area can be expected, especially in the area of novel magnetic fluids with liquid-crystal-like ordering.

Glasses and Amorphous Solids

The principal achievements in the fundamental understanding of this important class of materials has come from detailed measurements of the static structure factor by x-ray and neutron scattering, combined with the detailed information about local order derived from extended x-ray absorption fine structure (EXAFS). In particular, the use of isotopic substitution methods for neutron diffraction, combined with x-ray diffraction results, has led to direct determination of the partial structure factors for several glasses. This has provided a better understanding of the short-range structure and chemical ordering in a wide variety of glasses. However, much work remains to be done both on the intermediate-range structure and on the recrystallization process (using small-angle neutron scattering). Progress in this area requires exceptionally high-quality data extending over the widest possible range of momentum transfers, placing severe demands on instrumentation. The development of intense pulsed spallation sources will greatly enhance detailed analysis of interatomic arrangements in these systems.

To date, little work has been done on the dynamic properties of glasses, at least partially because of the lack of adequate theoretical models. Nonetheless, important results have been obtained on reasonably simple metallic glasses ($Ca_{10}Mg_{30}Zn_{30}$) and compared with computer simulation studies done using pair potentials derived from pseudopotential theory. These experiments have shown that the pair potentials used in the simulations give a good representation of the dynamics and have led to increased efforts to derive better potentials for semiconductors and insulators. New predictions

concerning phonon density of states in amorphous materials based on the fractal nature of self-similar structures need to be explored by neutron-scattering experiments. As these and other efforts continue, neutron scattering will unquestionably provide the ultimate test of most theoretical models, since it provides data over a uniquely wide range of energy and momentum.

NEUTRON OPTICS

A range of phenomena similar or analogous to those of classical optics is exhibited by slow neutrons. During the past 6 years considerable interest has been generated in this field from the point of view of fundamental physics. This has been due largely to the successful application of the perfect silicon-crystal interferometer to neutron experiments and to the increased availability of more intense sources of long-wavelength neutrons.

Neutron optical ideas and techniques play an important role in all aspects of neutron-scattering technology, in particular in the extraction, filtering, and monochromatization of beams. Substantial advances have been made in recent years in focusing monochromators, collimation systems, multilayer mirrors, and beam guides. We will not attempt to enumerate these advances in the application of neutron optics to neutron scattering generally but will instead discuss the variety of interesting experiments that have made an impact on our understanding of basic quantum-mechanical phenomena.

The Bonse-Hart perfect-crystal interferometer was first shown to work for neutrons by H. Rauch, W. Treimer, and

U. Bonse at a small reactor in Vienna, Austria, in 1974. It is topologically analogous to the Mach-Zehnder interferometer of classical optics. It consists of three identical perfect silicon-crystal slabs, cut perpendicular to a set of strongly reflecting lattice planes from a single monolithic crystal. The incident beam is coherently split and recombined by Bragg reflection. Alternative two- and three-crystal geometries have been employed successfully. In recent years, these devices have also been used at synchrotron radiation sources to measure the dispersion correction f` close to the x-ray absorption edges. These measurements of the real part of the forward-scattering amplitude directly reflect the EXAFS of the absorption spectrum.

In the neutron case, these devices have allowed the observation of quantum-mechanical interference phenomena on a macroscopic scale. They are extremely sensitive to very small potentials acting on the neutrons. The current level of sensitivity approaches 10^{-12} eV. Interference effects induced by the gravitational field of the Earth have been observed. In fact, the much smaller phase shifts due to the Earth's rotation (a quantum-mechanical analog of the famous Michelson-Gale-Pearson optical experiment) have also been observed. These experiments are the first tests of the principle of equivalence in the quantum limit. The first direct observation of the prediction that the operator for rotation through 2 rad causes a reversal of sign of the wave function for a fermion was also done with this device. A complete list of the experiments utilizing thermal neutron interferometry is now quite long. It includes the observation of the coherent superposition of spin states, study of the charge dependence of the four-body nuclear

interaction, search for quaternions in quantum mechanics, observation of the neutron analog of the Fizeau effect, search for nonlinear terms in the Schrödinger equation, measurement of the longitudinal coherence length of the neutron, and a search for a neutron Aharonov-Bohm effect. Interference in spin space, using the nuclear magnetic resonance-Ramsey technique, has recently been used to observe optical rotation via parity-violating weak interactions. While the perfect crystal interferometer utilizes interference by amplitude division, interferometers based on division of the wave front have also been successfully employed in recent years. In order to achieve a reasonable beam separation, these devices all utilize long-wavelength neutrons (` 20 Å) obtained from a cold source. The neutron Fizeau experiment was carried out using this type of interferometer. Many of the well-known optical phenomena have now been observed with neutrons, including two-slit interference (Young's experiment), operation of Fresnel zone plate lenses, thin-film multiple interferences, and diffraction by a straight edge. Cold neutrons have also been essential in recent experiments on the neutron lifetime and continuing searches for the electric dipole moment (EDM) of the neutron. Novel methods for producing ultra-cold neutrons involving Doppler-shifted Bragg scattering and downscattering in liquid helium have been demonstrated successfully in the last several years.

At present, fundamental physics utilizing neutron optical techniques is primarily carried out at four places: the University of Munich, the Institut Laue-Langevin in Grenoble, the University of Missouri, and the Massachusetts Institute of Technology. It is difficult to predict the future directions

that this field will take. However, there are various fundamental neutron-optics-related experiments currently in progress and others on the immediate horizon. It is likely that continuously higher-precision searches for a neutron EDM will be pursued using ultra-cold neutrons. The measurement of the energy dependence of neutron-scattering lengths using various interferometers will be pursued as these data become necessary for scattering experiments using epithermal neutrons from pulsed spallation sources. A Michelson-Morley experiment with neutrons should be done. Very small effects, such as the coupling of the neutron spin to the curvature of space-time (owing to the presence of the Earth), are in principle detectable with significantly larger interferometers, having linear dimensions of a meter or so. Neutron trajectory and effective mass experiments in dynamically diffracting crystals are in progress. Experiments related to fundamental temporal and spatial coherence questions and Wheeler's delayed-choice questions have just begun. The next 5 years will probably be as exciting as the past 5 years.

CHEMISTRY

Crystallographic Research

The years from 1977 through 1983 were active ones for structural studies using neutron diffraction, not only because of extensive work with single crystals but also because these years included vigorous growth in the application of high-resolution powder diffraction to structure refinement by means of the technique

in which the entire diffraction pattern is fitted to a detailed crystallographic model. This technique, which has become known as the Rietveld method, has revolutionized structure studies on both sides of the Atlantic for a wide variety of materials that are not available as single crystals. Moreover, the penetrating power of the neutron makes possible the study of crystal structure under extreme conditions of temperature and pressure. Materials that have received extensive attention include compounds that contain light atoms in the presence of heavy atoms, such as organometallic compounds and heteropoly complexes; ionic conductors; superconductors; both alloys and organic compounds; framework structures, such as zeolites; simple and moderately complex compounds in which neutron and x-ray data can be combined for studies of electron density; hydrogen-bonded compounds; magnetic compounds; and simple organic and inorganic compounds in which high-precision structure analyses can be correlated with physical properties or compared with ab initio calculations of expected molecular conformations. We discuss below particular examples of some of these types of structural study.

Hydrides, Organometallic Compounds, and Heteropoly Complexes

Because of its sensitivity to hydrogen and other light atoms in proximity to heavy metals, neutron diffraction has proved invaluable in studying the structures of transition-metal hydrides and metal complexes with organic ligands exhibiting C-H/metal interactions. Between 1977 and 1983 approximately 50 metal hydride structures have been investigated by single-crystal neutron techniques, providing examples of hydrogen in terminal, bridging, and interstitial environments. Many powder-diffraction studies of binary and ternary hydrides

have been carried out, including such potentially technologically important materials as $FeTiH_x$ and $LaNiH_5$. In studies of C-H/metal interactions, neutron diffraction has provided information on models for C-H bond activation processes that are of fundamental importance in catalysis. In recent years there has been increased emphasis on the study of cluster compounds, which may provide models for the bonding of hydrogen atoms and small molecules to metal surfaces. Crucial studies have also been carried out on heavy-metal-based heteropoly complexes, compounds of extensive importance as reagents and catalysts, which contain hydrogen as integral parts of the heteropoly anions.

Ionic Conductors and Ceramics

Studies of ionic conductors such as ß``-alumina, AgI, Ag_2S, Cu_2S, and related ternary systems, as well as $Na_{1-x}Zr_2Si_xP_{3`x}0_{12}$ (NASICON) and $Na_3Sc_2(PO_4)_3$, are of great interest and exploit the unique advantages of neutron diffraction, in combination with x-ray diffraction, for examining details of disorder and thermal motion. Another important class of ionic conductors contains lithium in a matrix formed by a refractory metal oxide. Neutron diffraction is the key to determining the critical role of Li and accurate oxygen cage geometries in such “electronic” ceramics (e.g., $LiReO_3$, $LiTaO_4$). Such new materials have great potential, for example, in the development of more efficient small batteries.

Superconductors

Neutron diffraction has played an essential role in providing a basis from which to understand the unusual properties of organic conductors and superconductors. For example,

in the partially oxidized tetracyanoplatinate complexes, the one-dimensional electronic conductivity has been studied as a function of metal-metal distance for a range of materials whose structures are known from neutron diffraction. More recent neutron-diffraction studies of organic, superconducting materials of the TMTSF family have explored the structure-property relationships that might exist between materials that exhibit superconductivity only at high pressure and materials that are superconducting on appropriate anion substitution. Neutron powder diffraction has been used to study a wide range of ternary superconducting alloys, in particular the Chevrel phase structures.

Framework Structures

Studies of zeolites are giving the first precise information on the locations of extra framework molecules and ions in these technologically important materials. For example, studies of zeolite rho with various compositions and over a wide range of temperatures have shown that this zeolite is noncentrosymmetric for most compositions. The sizes of the pores are sensitive to the degree of departure from centrosymmetry. These and other zeolite structure data are being used to test structural models of the reversible dehydration and ion-exchange properties of zeolite molecular sieves.

Charge-Density Studies

Techniques for combining high-resolution neutron and x-ray diffraction data to yield detailed information on electronic charge-density distributions in crystals have been extended from structures involving only atoms in the first row of

the periodic table to compounds containing heavier elements.

These studies are yielding important information on chemical bonding, including the distribution of d electrons in transition-metal systems.

New opportunities for understanding chemical bonding have been opened by the development of high-intensity polarized-beam diffractometers at the ILL, which are measuring the spatial extent of p and d electrons in complex chemical systems. Although these systems are not magnetically ordered in any sense, a strong magnetic field is used to induce a spin susceptibility. The results of such measurements, when combined with high-resolution neutron diffraction and x-ray results, can be compared with first-principle calculations of the atomic wave functions.

Hydrogen-Bonded Compounds

The study of the structures of hydrogenous solids has been one of the particular strengths of neutron diffraction ever since its early development in the 1950s, and interest in these compounds continues unabated. Particular attention has been directed toward the study of very short hydrogen bonds and the question of whether they are symmetrical. A number of cases have been found of very short hydrogen bonds that do not cross centers of symmetry, and these appear to be asymmetrical. If the crystal structure can be centrosymmetric, and if the distance between two oxygen atoms is shorter than about 2.45 Å, a symmetric O-H-O hydrogen bond is indistinguishable from an asymmetrical one with statistical disorder across the center.

High-Precision Structure Studies

The high precision currently available from neutron-diffraction structure analysis has made possible a variety of new types of studies--atomic positions may frequently be determined with a reproducibility of 0.001 Å or better. For example, investigations of a number of pyroelectric materials have shown that observed changes in polarization with temperature are consistent with the values calculated from the lattice constants and the nuclear positions. In another type of investigation, conformations of small molecules determined at temperatures about 20 K are being compared with those inferred from ab initio quantum-mechanical calculations. Such comparisons are providing insight into the distinction between effects intrinsic to the molecules and effects of forces in the solid.

Molecular Fluids and Molten Salts

In recent years, neutron diffraction work on “chemical” liquids has been carried out almost exclusively in Europe, where a sizable number of physicists and chemists, notably in the united Kingdom, have turned to liquid-state problems. In the united States, two small programs have concentrated on water and water-based solutions and on molten salts. It has now become clear that in order to unravel the structure of molecular fluids and molten salts, the partial structure functions descriptive of these systems must be resolved by multiple experiments with isotopically substituted samples. This requires elaborate sample preparation techniques and access to high-flux reactors or pulsed sources. The substitution method has been successfully applied to ions with isotopes having large differences in coherent-scattering lengths,

such as Ni, Nd, and Cl. The method can be extended to nuclides with small differences in scattering length such as ^{12}C and ^{13}C or ^{14}N and ^{15}N. However, the large-scale investigation of these interesting systems is at the edge of the capabilities of currently available neutron sources and would greatly benefit from an order of magnitude in intensity. Structural solution chemistry has already been revolutionized by the isotopic substitution method, which allows the unique determination of ionic hydration and of ion-ion pair distribution functions. The method will be extended to the study of molecular fluids.

In order to determine molten salt structure completely, both cation and anion isotopes should be available. Salts of the type MX and MX_2 have been systematically investigated, giving special attention to the role of ion size. Future work will focus on binary melts.

Chemical Spectroscopy

With neutron molecular Spectroscopy one may currently study the dynamics of molecules ranging from slow translational and rotational diffusion (10^{-6} sec) to the highest-energy internal vibrations (10^{-14} sec) at wavevectors (0.01-10 $Å^{-1}$), which directly probe molecular or macromolecular dimensions, something no other single experimental technique is capable of. However, most of this range is inaccessible with instruments at present U.S. neutron sources, as we will discuss in more detail below. Consequently, activities in this field in the United States have been somewhat limited.

Vibrational Spectroscopy

Current U.S. research efforts in neutron molecular spectroscopy are concentrated on vibrational spectroscopy in the range 25-250 meV using recently developed specialized instrumentation at reactors and pulsed neutron sources. Unlike most other spectroscopic techniques, incoherent inelastic neutron scattering (IINS) is not governed by symmetry-based electromagnetic selection rules. Instead the amplitude of the vibrational mode and the nuclear-scattering cross section of the atom involved principally determine IINS intensities. These factors favor the motions of H-atoms, and, therefore, certain kinds of normal modes (e.g., methyl torsions), which are often inactive or weak in IR or Raman scattering, have very large intensities in IINS.

Most (but not all) of the work in this field has, therefore, concerned hydrogen-containing molecules and has often played a crucial role in assignments of vibrational bands when used in conjunction with light scattering. For example, a series of experiments on compounds with very short hydrogen bonds using IINS measurements demonstrate an apparent change in the dynamics of the O-H-O bond as the O-O distance r becomes less than about 2.44 Å. This was accomplished by measuring the out-of-plane bend (OHO) as r decreases. It had been impossible to assign this mode in light-scattering experiments. Other cases for which IR/Raman spectroscopy is often difficult or impossible include metallic systems, some intercalated species, and inorganic complexes that fluoresce. Moreover, recent work at both U.S. and European reactors has shown that IINS provides a powerful, often unique tool for in-situ spectroscopy of chemisorbed species

on catalysts over a wide range of temperature and pressure. These studies have already provided direct information on the bonding states and interactions of H atoms on the surface of Ni and Pt particles and on adsorption and decomposition of organic molecular species on these catalysts. An important advantage of IINS in such studies is that the scattering can be described by relatively simple theory, so that spectral intensities can be used quantitatively in the interpretation of spectra. For example, in the spectroscopic work on catalysts, both vibrational peaks and intensities were used to determine the geometry and force constants of surface-bound species. A series of important experiments has also been performed (in Europe) on metal cluster compounds as analog systems of chemisorbed materials. These data are extremely valuable as an aid in interpreting neutron or optical spectra of species bound on (or in) a real catalyst.

Low-Energy Spectroscopy

Low-energy neutron spectroscopy is currently done almost exclusively in Europe, where a series of specialized spectrometers has been developed over the past 5 or 10 years, primarily using cold neutrons, which have expanded the spectral range of neutron scattering by up to 5 orders of magnitude (down to 10 `^{9} ev). These include superior, highly sensitive cold-neutron time-of-flight spectrometers, as well as ultra-high-resolution backreflection and spin-echo spectrometers. This capability, combined with the unique wave-vector regime available with neutrons, has opened up entirely new and exciting areas of applications of neutron scattering, not only in chemical spectroscopy but, as reflected in other

sections of this report, in condensed-matter physics, polymer science, and biology.

In chemical applications, low-energy neutron spectroscopy is an extremely sensitive tool for probing the intermolecular potentials and the details of rotation and diffusion of molecular species in condensed systems. For example, neutrons can be used to measure rotational ground-state splittings (tunneling) by spin-flip scattering. These transitions are between different nuclear spin states and, therefore, forbidden in light-scattering studies. Such measurements most often require ultra-high resolution (European instruments for this purpose have achieved 0.5-μeV resolution), but some work has been attempted at U.S. reactors on triple-axis spectrometers at relatively low resolution (~50 μeV).

Perhaps the most notable such example is a study of NH_3 rotations in $Ni(NH_3)_6I_2$, where both the form of the orientational potential and (by the application of hydrostatic pressure) its approximate dependence on intermolecular distance could be determined. Similar work was carried out on nitromethane and methane but could only be completed by making use of the appropriate instruments at the ILL. Thus the entire field of rotational tunneling spectroscopy, including appropriate theoretical advances, has been developed in Europe since the mid-1970s. Perhaps the most impressive example is a series of experiments and calculations on tunneling states in methane as well as its deuterated forms. In the low-temperature phase III of CD_4, e.g., eight transitions were resolved in the range 0-8 μeV on the IN-10 spectrometer at the ILL. This work has led to a detailed understanding of quantum-mechanical rotations and intermolecular potentials in the solid methanes. In an extension of this work to

methane absorbed on graphite, it was possible to determine the relative importance of molecule-molecule and molecule-substrate forces by comparing tunneling levels for various types of rotations of the molecules on the surface. We should like to stress that this type of low-energy spectroscopy, when combined with IINS vibrational spectroscopy, provides a powerful and comprehensive probe for studying molecule-surface interactions.

The same general comments apply to the study of rotational and diffusive molecular motions with relatively long time constants (10^{-10} sec) by quasi-elastic neutron scattering (QNS). This is a powerful method for studying such motions in a wide variety of systems, ranging from hydrogen diffusion in metals to relaxation processes in polymers. Because of the ability to measure QNS at different momentum transfers, one can determine the details of reorientation or diffusion mechanisms on an interatomic or molecular scale. The application of these techniques and the development of advanced high-resolution neutron-scattering instruments is expanding rapidly in Europe. In fact, QNS has become a heavily utilized probe for investigation of molecular motion and diffusion in homogeneous as well as heterogeneous systems, such as zeolites, clays, clathrates, and other chemical adsorbents and intercalated materials. Measurements have been extended down to less than 1 atomic percent of molecular species.

BIOLOGY

Most of what we know about biological structures comes from the observation of radiation scattered by objects. Visible

and infrared light, electrons, and x rays have provided structural information ranging from the organization of the atoms in macromolecules to the arrangement of cells in organisms. With the development of high-intensity sources and improved instruments, it has recently become possible to use neutrons as an additional form of radiation with which to study the structure and dynamics of macromolecules and molecular assemblies.

Neutrons have different scattering properties compared with the other forms of radiation that have been used and therefore can reveal different aspects of structure and, in fact, have capabilities that are uniquely useful. Isotope effects, particularly the difference between hydrogen and deuterium, can be exploited by selective labeling of the molecules of interest or of the solvent. An additional advantage is that there is no radiation damage to the specimen. Finally, neutron inelastic scattering provides the possibility of probing low-energy states of motion in biomolecular structures.

The principal biological areas in which neutrons have been applied during the past decade have been in high- and low-resolution macromolecular crystallography, in studies of molecular assemblies and molecules in solution, and in the study of some partially ordered systems. In all cases the difference between the scattering of hydrogen and the scattering of deuterium has been used as an important tool. In studies of protein crystals, for example, the location of hydrogen atoms (which are not observed in x-ray crystallographic experiments) has been studied, and their replacement by deuterium has led to ideas concerning structural dynamics. Moreover, crystallographic studies at low resolution

have exploited enhanced contrast between protein and nucleic acid components of macromolecules. Specific deuteration of parts of macromolecules or macromolecular assemblies has been used to extend the range of information that can be obtained from solution scattering measurements. Similarly, studies of biological membranes and related lipid systems have provided critical information beyond that obtainable by x-ray diffraction. In the following, several examples of biological studies are discussed.

Protein Crystallography

High-resolution protein crystallography with neutrons was first attempted in Europe in the early 1960s but became truly feasible only in the mid-1970s. Currently the major facilities capable of efficient data collection exist in the United States, and a comparable facility is close to completion at ILL. Low-resolution studies of single crystals of such assemblies as nucleosomes and viruses have been attempted only at ILL and have never been performed in the United States, primarily for lack of suitable instrumentation.

Studies of protein crystals using neutron diffraction at a resolution of 2 Å or better have focused on the localization of hydrogen atom positions and on the exchange of hydrogen for deuterium. By documenting the position of hydrogens, it is possible to understand more completely the chemistry of proteins, which often involves hydrogen atoms in critical roles. Examples of such studies are myoglobin, trypsin, ribonuclease, lysozyme, and crambin. Studies of trypsin and myoglobin led to the elucidation of the location of individual hydrogen atom crucial to the activity of each

of these proteins, while unexpected results concerning the details of hydrogen bonding between the enzyme and a substrate analog emerged from the analysis of ribonuclease.

A second line of crystallographic studies has been to follow the exchange of hydrogen and deuterium, using the exchange patterns to derive ideas concerning the distribution of static and dynamic regions of the structure. Examples in which important information has been gained are ribonuclease, trypsin, and myoglobin. Certain structural regions have been found to be relatively stable, at least so far as the dynamics of a molecule in a crystal are concerned. Continuation of these studies is anticipated and may shed important light on the dynamics of proteins and, possibly, other macromolecules. Of particular importance may be the comparisons with the dynamic results obtained by NMR.

A third issue that has concerned the practitioners of neutron crystallography has been the interaction of macromolecules with the solvent environment. Using neutrons, it is possible to document the occurrence of bound water molecules with much greater assurance than is the case with x rays, and ideas about solvation of proteins have emerged from such studies.

It is clear that high-resolution neutron crystallography has been an important and productive development as applied to biological macromolecules. It is expected that contributions from this approach will continue in the future and that a number of important biological issues may be addressed in the areas of protein structure, enzyme mechanisms, protein dynamics, and solvent interactions.

Low-resolution (15 Å or lower) studies in Europe utilizing contrast variation have been performed on a number of assemblies

consisting of proteins and nucleic acids. Such studies are capable of delineating precise boundaries between the components and are useful if high-resolution data cannot be collected. The instrumentation is provided by modification of modern small-angle instruments, which must be equipped with large area detectors and have access to cold neutron beams (~10 Å).

Solution Scattering

This technique has been found to be of great importance in studies of biomolecules consisting of components that could be selectively masked by the use of appropriate H_2O/D_2O solvents. Instruments capable of necessary measurements are now available on a number of reactors in this country and in Europe, although the best European instruments have higher flux and are capable of lower wave-vector measurements, which permits examination of larger structures.

A number of different assemblies have been studied in solution using neutron scattering. Significant findings concerning nucleosomes, viruses, lipoproteins, ribosomes, and other systems have been derived from studies in both Europe and the United States. We will now discuss an example of such studies.

The Ribosome

More than 10 years ago, it was proposed that the organization of the proteins in a ribosome could be determined using neutron scattering from ribosomes in solution. The basic idea was to place two deuterated proteins in an otherwise hydrogenated structure. Neutron scattering from solutions

of such labeled particles could then be used to obtain a measurement of the distance separating the centers of the two proteins in question. By a process of triangulation, a three-dimensional map of the positions of proteins in a complex structure can be generated. Such a map will be extremely useful in understanding functional relationships of different parts of the ribosome structure. In 1974, the first measurement was carried out. Since then, a large number of pairwise measurements have been made, and the positions of 15 of the 21 proteins of the small subunit of the E. coli ribosome have now been established. Once a map is obtained, the positions of other macromolecular ligands can also be investigated, as can issues concerning conformational changes that may accompany different states of activity.

Partially Ordered Systems

Partially ordered systems, particularly those involving membranes or muscles, for example, can be investigated using the same instrumentation as the solution measurements, although more specialized instruments for low-resolution crystallography have been and are being developed. Membranes, such as those of the myelin sheath, sarcoplasmic reticulum, retinal rod, and halobacterium, have been studied. Furthermore, details of lipid bilayer structure have been documented using deuterium labeling of specific sites.

An example is bacteriorhodopsin, a small protein found in crystalline patches in the plasma membrane of a microorganism. The protein is responsible for converting incident light energy into energy stored in an electrochemical gradient

across the membrane of the organism, which it does by pumping protons from the cytoplasm to the outside in response to light. Understanding its structure may lead to improved ideas concerning the nature of membrane proteins and their relationship to lipid bilayers, as well as leading toward an understanding of the energy transduction process itself.

The neutron-scattering approach has been to use specific deuteration of the molecule by providing deuterated amino acids in the growth medium of the organism. In this way, individual classes of amino acids in bacteriorhodopsin can be deuterated biosynthetically. Purple membranes are then isolated from the organism, and their diffraction of neutrons is measured. Deuteration of different amino acids leads to large intensity changes, which can then be used in a model-building approach to test choices for the organization of the structure. This work is now in an advanced stage, and two of the seven helices have been assigned. Furthermore, it has emerged from this and other work that the helices are oriented so as to place polar groups toward the inside of the protein and nonpolar groups toward the outside where they may make contact with the nonpolar region of the liquid bilayer. Thus, this membrane protein is "inside-out" when compared with the normal organization of soluble proteins.

It is to be expected that further study will lead to more refined techniques of labeling and measurement and to corresponding improvements in the views of biological structures derived from partially ordered structures.

Inelastic Scattering

The application of inelastic scattering to biological studies has only just begun. After a number of efforts in Europe, a start has been made in developing both the theoretical framework and the measurement techniques that will be needed for biological studies. An example of the work carried out so far is a study of the enzyme hexokinase, which changes its conformation when it binds one of its substrates, glucose. In a series of measurements in D_2O solvent systems, French scientists have succeeded in demonstrating a change in the dynamics of the hexokinase molecule when glucose is bound. Such dynamic changes may accompany many instances of enzyme-substrate interactions and could be useful in probing the dynamic interdependence of multicomponent systems as well.

The development in the United States of suitable instrumentation for low-energy (0-10 meV) neutron spectroscopy, competitive with the best European facilities, would permit an evolution of this potentially exciting area of biological study.

Conclusion

The applications of neutrons in biology have led to important new insights concerning membrane proteins, enzymes, the ribosome, nucleosomes, the organization of lipid bilayers, virus structure, nucleic acid-protein interactions, and many other areas. It is clear that, while the techniques may appear exotic and specialized to biologists, essential and unique information is gained. There is every expectation

that such gains will continue to grow in the future, as improved instrumentation and new sources are developed.

POLYMER AND COLLOID SCIENCE

The availability of SANS facilities has led to revolutionary advances in polymer science over the past decade. The substitution of deuterium for hydrogen makes it possible to extract information about the global molecular geometry of polymer molecules in the presence of high concentrations of other polymer molecules of the same chemical structure but differing isotopic composition. There are no other experimental methods for making such measurements. Results already achieved have stimulated significant theoretical advances, which, in turn, have given direction to many new experiments.

These determinations of molecular geometry are derived from the coherent, elastic component of the scattering envelope. Since polymer molecules are large, it follows that experiments at low q are of greatest significance.

Quasi-elastic scattering has played a lesser role in the study of polymers. This is partially due to the uncertainty in the theory used for interpretation and partially due to the inaccessibility of suitable instrumentation. The “best” spectrometer of this sort, the spin-echo machine at ILL does not go to sufficiently low q to be completely satisfactory. The problems that can be solved uniquely by quasi-elastic scattering are manifold, and the results are a natural extension of information obtained by other methods. Inelastic neutron-scattering measurements of the

higher-energy frequency dynamics of polymers can also be quite valuable. A complete analysis requires large deuterated single-crystal samples, which are usually not available, but determination of large-amplitude modes (e.g., torsions) and density of vibrational states by incoherent scattering yields information complementary to that obtained by optical spectroscopies.

Since most of the research in the recent past on high polymers has been conducted for the purpose of the study of molecular geometry, we concentrate primarily on coherent elastic low-angle neutron scattering. The application of quasi-elastic scattering of polymers is at an earlier stage of development and will be discussed more briefly.

Areas of Special Interest

Polymer molecules are long-chain structures that are largely coiled, with molecular weights varying roughly between 10^4 and 5×10^6 and having a characteristic linear dimension, the centroidal radius of gyration (R), lying between 25 Å and 800 Å. In most cases, data obtained in a range between $0.3 \grave{} qR \grave{} 5$ are adequate, which means that for the large molecules a minimum q (momentum transfer) of $4 \times 10^{\grave{}4}$ Å$^{\grave{}1}$ is desirable, and for smaller molecules the largest q required would be 0.2 Å$^{\grave{}1}$. It is difficult to do experiments at low values of q at sufficiently high flux, and this has caused researchers to avoid polymer systems in which molecular weights are greater than 300,000.

In many cases, with polymeric electrolytes, for example, it is desirable to work at low polymer concentration, less than 1 percent by weight. The errors owing to low signal/noise

ratios are considerable in systems of such low concentration, and the time for a single experimental run becomes unreasonably long.

The dimensions of particles in colloids are comparable with those in polymers, contrast is established by substitution of deuterium for hydrogen, and therefore the SANS requirements are of the same kind. One difference is that colloidal particles are compact, while polymer molecules are normally somewhat extended. As a result, the scattered signal from colloids is more intense, and experimental limitations tend to be less stringent. Quasi-elastic neutron scattering is used for examination of local motions such as methyl group rotation, polymer diffusion, and global dynamics of polymer molecules. The study of global dynamics is most demanding, and this aspect of polymer motion cannot be probed easily by other methods. Generally, the interest is in low-frequency motions in which long sections of the polymer molecule move in concert. The current instruments provide data at low frequency (down to 10^6 Hz) but are signal limited to q's greater than 0.02 $Å^{-1}$, and this is not yet low enough to characterize chain dynamics fully. The limitation on q should be addressed in the development of new higher-q resolution spin-echo spectrometers.

Some Results from Neutron Scattering

The overall chain conformation of a polymer molecule in the bulk had been assumed alternatively to be (a) a random coil with no measurable excluded volume repulsive effects or (b) an ordered structure with neighboring chains strongly influencing mutual conformational arrangements. In the

absence of SANS, it was not possible to distinguish between these alternatives. SANS measurements on a number of systems strongly support assumption (a), a conclusion that is now accepted universally. While the bulk state is important, it is only one line on the temperature-concentration (T-C) map of a polymer system. Most polymers are synthesized or processed under varying T-C conditions. SANS has made it possible to study the molecular behavior at these conditions. Although most measurements were made in Europe, scientists from the united States have also made major contributions in this area. Moreover, some of the modern theoretical predictions (renormalization group calculations and scaling theory, for example) have been critically compared with conventional theories (mean-field theory and perturbation theory, for example). Advancement in this area so far has mainly been due to comparison with the SANS results. Dynamical studies in this area would be greatly advanced if high-flux, small-angle spin-echo instrumentation and backreflection spectrometers became available to U.S. scientists.

The verification of the kinetic theory of rubber elasticity, a theory based on analysis of chain statistics, has been dependent on measurements of network swelling and stress-strain behavior. SANS measurements make it possible to study the deformation of the molecular chains directly. Indeed, it has already been shown from SANS that chain deformation is substantially less than predicted. While this result has been criticized as arising from improperly prepared materials, it has provoked new efforts to improve the theory. Certainly, further measurements of this kind can be expected to stimulate new interest in the molecular theory of elastomers.

Block polymer molecules contain within a single polymer chain at least two different chemical subchains. In some interesting cases, these subchains separate into two microphases owing to mutual incompatibility of different parts of many molecules. These microphases are compact, each unit containing parts of many molecules. This is a colloidal-type structure of characteristic dimension 100 Å or so. Much attention has been given to these block copolymers owing to both their theoretical interest and to their significant practical applicability. They can be and have been studied conveniently by small-angle neutron scattering in which one of the blocks is labeled by deuterium. In a few cases where this has been done, it has been possible to decide which of several theoretical analyses is preferable.

Molecular conformation in binary systems and kinetics during phase decomposition is an important area in terms of future polymeric materials. Although it is still in its infant stage, it is already clear that neutron scattering will be one of the most important tools in this area. A high-flux, low-q SANS instrument with time-resolved measurement capability will be especially valuable. This is because the kinetics of microphase decomposition will be the major factor that controls the morphology and performance of the material. Thus, it will be of great scientific and technological interest to study the molecular details of phase decomposition kinetics.

Instrumentation Needs

Small-angle neutron scattering of high polymers and of colloids has become an essential research tool. More than 100 experimental studies have been published, the majority using neutrons from the D11 SANS facility on a cold-neutron guide at the ILL. The largest concentration of polymer and colloid work in the United States has been done during the past three years at the NSF facility at Oak Ridge, but important contributions have been made by researchers at the National Bureau of Standards, the University of Missouri, and Brookhaven National Laboratory. In Europe, SANS experiments have also been performed at Jülich, Saclay, and Harwell.

Most modern instruments have two-dimensional detection, in which case scattering-intensity problems are less with isotropic materials than with oriented samples such as fibers, stretched rubber, or stretched plastics. This is a consequence of the fact that intensities for anisotropic materials are measured over a narrow azimuthal range, and much longer experiments are needed. It is significant that almost all results on anisotropic scattering have been reported from ILL, where fluxes are an order of magnitude greater than elsewhere. Similarly, studies on polyelectrolytes are most interesting at low concentration (one percent by weight or less), and reliable results from such weak scatterers require higher fluxes than are currently available.

The needs for the future are clear. Higher neutron fluxes and an ability to attain a lower range in q are needed. With existing U.S. reactors, this could be obtained by use of a cold source and a monochromator of the velocity selector type. A guide hall adjoining the reactor building would

be needed for optimal resolution and flexibility. Recent work in Japan has demonstrated that useful research on some problems can be done at modest-flux pulsed sources equipped with a cold source. The possibilities for using the pulse structure of such sources in time-dependent studies will provide new opportunities when much higher-flux sources are developed.

Future needs for quasi-elastic scattering of polymers are focused on the problem of chain dynamics. The most promising spectrometer for this work is the "spin-echo" instrument, which permits a much better energy discrimination in the low-energy range than is otherwise obtainable. Thus far only a small number of experiments on polymers have been performed on the only spectrometer of this kind in use. However, the uniqueness and importance of the dynamical information that can be obtained from such measurements makes the construction of such facilities in the United States critical for research in polymer and biological systems. State-of-the-art cold-neutron time-of-flight and backreflection spectrometers would also make major contributions to future studies of polymer dynamics.

MATERIALS SCIENCE AND ENGINEERING

Neutron scattering offers a unique method of studying the response of materials to external variables such as stress, strain, temperature, and processing variables. The penetrating power of a neutron beam permits the sampling of a large volume of specimens, so that the investigation of bulk properties is possible. The energy of the neutrons is sufficiently

low that the testing procedure itself does not introduce any additional damage, as may occur with electron microscopy. The sensitivity of SANS to heterogeneities in the size range from a few nanometers to about a micrometer has made it possible to follow, often in detail, microstructural changes in metals and ceramics resulting from deformation, irradiation, or processing. The appearance or dissolution of carbides, precipitates, dispersoids, voids, and microcracks, for example, can be detected, and frequently with sufficient sensitivity and precision that the kinetics of the process can be ascertained and compared with theoretical models. In many cases, the information yielded by neutron scattering on material behavior can be obtained in such detail and with such accuracy by no other method currently available.

Studies of Microstructural Changes Produced by Temperature and Deformation

It was demonstrated several years ago in Europe that SANS has the potential to monitor thermal processing of complex alloys. Little work has been done to date in this area in the United States. Recently, a SANS study has been carried out to investigate the effect of austenitizing and aging conditions on the size and density of precipitates in a precipitation-hardening high-strength low-alloy steel. The results were correlated with mechanical behavior. A study such as this can be used not only to optimize processing variables but also to determine the allowable leeway in these variables before serious degradation of mechanical properties results. SANS has been used to follow microstructural changes produced by prolonged exposure to high temperatures

in a ferritic stainless steel developed for use in power-generation applications. Extended service causes microstructural alterations, which affect the mechanical properties of the steel such that it may no longer meet design requirements. Scattering experiments have given detailed information on the size and number of carbides ultimately produced at various temperatures. Deformation greatly hastens the microstructural changes associated with aging. Such changes were clearly picked up by SANS in steel samples fatigued for only a few hours. It may be concluded that service-induced microstructural changes can be detected and even analyzed in detail by SANS, even in complex alloys.

In Europe a number of investigations have been carried out in deformation-induced changes in microstructure. Advantage has been taken of the high-flux densities available in order to obtain small-angle scattering patterns over sufficiently short time intervals that the changes can be followed in situ. It should be noted that the scattering features of interest in metallurgical and ceramic studies frequently are rather large (some tens of nanometers). Their density is likely to be low. These are conditions that necessitate high-flux densities and measurement at very low values of the scattering vector. Such requirements cannot always be satisfied at U.S. facilities.

Use of SANS in the Detection and Analysis of Damage

Several recent experiments have pointed up the value of neutron scattering in the study of damage that appears in the form of cracks or voids. The ability of SANS to provide statistical information on the number, size, and shape of

microcracks has been demonstrated in an elegant investigation of the ceramic $YCrO_3$, which undergoes extensive microcracking when it passes through a phase transformation at about 1100°C. It was found that the small-angle scattering cross sections from the cracked $YCrO_3$ could be fitted well by the form of the scattering expected from an ensemble of randomly oriented thin disks. By combining the SANS results with data on the elastic constants of the $YCrO_3$, it was possible to determine the number density, average size, and shape of the cracks.

Grain-boundary cavitation is a phenomenon found in many metals and ceramics subjected to deformation at elevated temperatures. It was virtually impossible to examine the details of this process until the advent of SANS made available statistical information on the kinetics of void nucleation and growth. It has been found that most of the voids produced by fully reversed cycling are surprisingly small (about 35 nm). At this size they should not be stable against surface energy forces. Void volume fractions of less than 10^{-6} can be measured and cavitation picked up by SANS after only 15 sec of fatiguing. No incubation time appears necessary for void nucleation. Since fatigue produces large numbers of small voids it is just possible to carry out SANS studies in facilities currently available in the United States (although higher-flux and lower-q limits would improve the results).

However, the void nucleation rate in creep is low, whereas the growth rate is high. Therefore, successful creep cavitation studies by SANS demand the high-flux and low-q capabilities of the D-11 instrument at ILL and are not now feasible in the United States. Recent results on crept Cu from ILL

measurements show that, in contrast to the case of fatigue, no voids can be detected with sizes below the predicted value of the smallest stable void. As in the case of cyclic loading, no incubation time appears to be required for void nucleation. The measured void size distributions that evolve as creep proceeds have been modeled with remarkable accuracy on the basis of one of the well-known theories of void growth.

The theory generally believed to be applicable for these experimental conditions was found to give poor agreement with the SANS results. This is the first instance in which such a precise comparison between theory and measurement of grain-boundary cavitation has been possible.

Measurement of Texture and Residual Stresses by Neutron Diffraction

X-ray diffraction techniques are well developed for the measurement of both texture and residual stresses. However, the limited penetrating power of x rays has restricted the determination of these quantities to surface layers. Measurement of bulk properties has required destruction of the sample. The x-ray methodology can be applied to neutron diffraction to permit the nondestructive evaluation of texture and residual stresses as a function of depth from the surface. This use of neutron diffraction has great potential.

Several investigators have demonstrated that neutron diffraction can indeed be used to determine both texture and residual stresses throughout a component. Test pieces with known stress fields have been examined and satisfactory agreement found between measured and calculated values.

The method now has been applied to the determination of stresses in a number of situations, e.g., in depleted uranium and in composites in cemented carbides. In the latter case, evidence was found of large hydrostatic components of stress between carbide and binder, which arise because of significant differences in their coefficients of thermal expansion. The stress is relaxed by creep or fatigue. Recent measurements have shown that pulsed-neutron time-of-flight neutron diffraction also can be used to investigate residual stresses. Grain interaction stresses in a deformed polycrystalline alloy were determined and found to be in accord with model calculations. (X-ray techniques are not suitable for measuring nonuniform stresses that have a wavelength on the order of the grain size.)

Investigations of Phase Decomposition

SANS has proved to be a valuable tool in the study of precipitation phenomena, particularly spinodal decomposition. Information on the kinetics of decomposition has been obtained by following changes as aging proceeds in the maximum scattering cross section and the corresponding value of the scattering vector. Several investigators are studying spinodal decomposition in the FeCr system. A coexistence curve determined from scattering patterns was found to be consistent with a curve deduced from reversion experiments but considerably different from calculated values.

The high flux at ILL has permitted in situ observations to be made of the growth (or dissolution) of metastable precipitates. From the SANS data it was possible to determine whether zone formation at a given aging temperature took

place by nucleation and growth or by spinodal decomposition. In another recently reported in situ experiment at ILL, solute partitioning occurring during unmixing of a ternary alloy was studied. Three isotopes of one of the constituents were used in order to obtain independent scattering contrasts.

6.

FUTURE OPPORTUNITIES: FACILITIES AND RESEARCH

Based on the preceding scientific summaries, a number of needs and opportunities for U.S. neutron-scattering research are clear both in the short term and the long term. There is an immediate and critical need to develop state-of-the-art facilities in the United States to match and, where possible, extend the major instrumentation advances that have been made at research reactors in Western Europe in recent years and that have opened up entirely new areas of important scientific applications for neutron scattering. At the same time, it is essential to initiate without delay design studies for next-generation sources to assure long-term U.S. capabilities.

The best U.S. reactor sources provide immediate potential, not only for greatly expanded, internationally competitive facilities for cold neutron research on materials but also for new high-intensity, high-resolution thermal neutron instruments. This would involve the application and further development of cold-neutron-source and guide-tube technology to allow high-efficiency transport of neutron beams to large guide halls and provide maximum flexibility for new instrument development. It is also essential to pursue advances in supermirrors, polarization techniques, focusing monochromators and collimators, and area detector systems to optimize the sensitivity of this new instrumentation. It should be noted that research and application in virtually all of these areas, along with time-focusing and correlation techniques

for time-of-flight applications, are necessary for the successful development of a new generation of instruments at both steady-state and pulsed sources. Moreover, a healthy and fully competitive U.S. program in neutron-scattering research at existing sources can be achieved by an incremental funding increase that is a fraction of the current massive difference in operating funds and capital investment between the united States and Europe. The Japanese have already mapped out an ambitious program to bridge the even greater gap in neutron-scattering capabilities that they face relative to the Western Europeans.

As pointed out in the scientific summaries, the development in the United States of new high-resolution, high-sensitivity instrumentation, and its utilization at both existing reactors and next-generation higher-flux sources, would provide major new scientific opportunities in all areas of neutron-scattering research, opportunities that are impossible to pursue by any other technique. The following provides both general and specific examples of these opportunities, which in some cases extend or summarize items discussed in Chapter 5.

CONDENSED-MATTER PHYSICS

The increased introduction of multidetector systems will greatly facilitate the search for diffuse scattering and weak satellite reflections in novel systems (e.g., charge-and spin-density waves). Moderate-resolution time-of-flight instruments of sufficiently high sensitivity at cold-source guides will permit studies of dynamics of physisorbed and intercalated atoms and molecules. Although it is anticipated

that much of the spectroscopy at energies of 100 meV or higher will be performed on pulsed sources, the study of strongly dispersive high-energy excitations (e.g., high-energy spin waves, Stoner excitations) may often be done best at a steady-state source equipped with a hot source.

The development of high-resolution spin-echo and backscattering spectrometers will open new regimes in the study of slow phenomena, such as relaxation effects in glasses and viscous fluids, spin glasses, and random magnets. Diffusion of hydrogen in metals, charge transport in ionic conductors, two-dimensional diffusion of intercalates in layered lattices, and rotational tunneling in molecular crystals are further examples of studies that will greatly profit from such instrumentation. With further technical advances in momentum focusing, these instruments would also be capable of high-resolution phonon linewidth studies, which would revolutionize our capabilities in addressing anharmonic effects, particularly with regard to electron-phonon interactions in superconductors.

The use of spin-polarized neutron beams for scattering experiments has always been limited by low neutron fluxes. This is often because exotic materials unfortunately are usually available in very limited sample size in the vital initial phases of their characterization. An elegant class of experiments requiring analysis of the polarization of the scattered neutron beam has always been severely limited by low flux. The development of higher-flux sources and more efficient and versatile polarizers would permit this technique more nearly to approach its true potential. Among the important experiments in this area are studies of spin fluctuations in paramagnets, separation of transverse and longitudinal excitations in itinerant magnets, and the

characterization of the nature of the ordering and excitations of materials undergoing cooperative nuclear spin orientation at low temperatures.

CHEMISTRY

Most of what has been accomplished to date in neutron spectroscopy of molecules in condensed systems has only scratched the surface of what it is possible to do with neutrons in this area--this will clearly be one of the major growth areas of neutron-scattering research in the future. The development in the United States of high-resolution, low-energy spectroscopy instrumentation, which provides perhaps the most unique information with respect to other methods, is a particularly critical need. It would open up for the first time in this country detailed studies of tunneling phenomena, rotational processes, and diffusion in molecular solids and in molecules bound in homogenous and heterogeneous chemical media. At the same time, the U.S. pulsed-source effort combined with existing reactor instrumentation can provide the higher-energy vibrational spectroscopic capability that is needed. The special sensitivity of neutrons (e.g., to H atom motions in optically opaque media) and the ability to interpret spectroscopic intensities directly provide unique opportunities in a number of areas. A more unified approach in the use of quasi-elastic, low-energy rotational and vibrational spectroscopy will be needed to achieve a full understanding of molecular dynamics, interactions, and bonding in a number of systems (e.g., chemical adsorbents and catalysts, intercalated materials). It should

be noted that much of future activity in neutron chemical spectroscopy will involve the use of difference spectra and isotopic substitution, where the signal from the species of interest is small compared with that from the surrounding media. This, combined with the fact that often the sample sizes available for spectroscopic studies of new novel compounds are very small, will require development of much more sensitive instrumentation and higher-intensity sources than are currently available.

In the area of chemical crystallography there is a great opportunity by a combination of increased flux (from more intense sources) and the use of area detectors, which would provide up to a factor of 100 improvement in sensitivity, to expand the range of applications of neutron diffraction to new classes of materials, e.g., inorganic complexes and ceramics, which are only capable of growth as very small (<1 mm^3) single crystals. As another example, such increases in data rates would also open up new applications of neutron diffraction for real time (~1 sec) in situ studies of solid-state chemical changes occurring during the processing of bulk ceramics, including new kinds of “electronic” refractory materials.

BIOLOGY

Future opportunities for biological research fall in the areas of crystallography, solution studies, and molecular dynamics.

Neutron crystallography at high resolution has been well developed in studies of small proteins but would greatly benefit from higher-flux sources to allow extension to larger

proteins, which must be explored to probe fully the structure of biological systems. Low-resolution crystallography clearly requires improved instruments and higher-flux sources of subthermal neutrons. There are no low-resolution, cold-source-based diffractometers in the United States that are comparable with the instruments available in Europe, and almost all of the major contributions in this area (nucleosomes, purple membranes, and virus structure) have emerged from recent studies at the Institut Laue-Langevin. In this regard, the possibility of combining low-resolution crystallographic and solution scattering measurements using a single instrument should be explored.

Solution studies have been and will continue to be important, owing to the unique structural information provided by the hydrogen-deuterium contrast. However, there is a critical need of improved instruments for operation at long (2-15 Å) wavelengths and higher fluxes. It is significant to note that, at wavelengths in the 5 Å region, the D11 instrument in Grenoble provides an intensity more than an order of magnitude higher than any U.S. instrument. Such gains in flux or resolution or both would open up in the United States applications to a wide range of biological problems, which cannot now be approached.

Finally, it should again be stressed that the exciting potential of neutron inelastic scattering in the study of low-energy relaxation and chain dynamics in biological assemblies can only be fulfilled if modern high-sensitivity cold-neutron time-of-flight and spin-echo instruments are developed in the United States.

POLYMERS

As summarized in Chapter 5, many fundamental questions that are also of technical importance in the polymer field could be answered if low-wave-vector (q) and very-high-resolution elastic and inelastic neutron-scattering instruments using high-intensity cold-neutron beams are made available in the United States. For example, in the area of polymer dynamics, quasi-elastic neutron-scattering instruments covering an extended q range (0.01 Å`1 ` q ` 2 Å`1) could provide an integrated understanding of the high-frequency motions that determine the chemical and electrical properties of polymers and the low-frequency (long-wavelength) motions that dominate the mechanical and transport properties. Neutrons can have a unique and critical role here by allowing a definitive test of various theories of polymer dynamics and relaxation phenomena.

The development of advanced high-resolution and high-intensity SANS instruments will also allow time-resolved measurements of changes in the molecular conformation and microstructure in polymer systems. An example would be studies of polymer chains under external stress either by steady-state or oscillatory shear or extension of the sample, with SANS observations made along the stress direction or phase locked with the oscillatory motion. Other important time-resolved measurements would also be opened up by state-of-the-art SANS instrumentation and higher-intensity sources, including studies of polymer phase decomposition or chemical reactions. There is also a great need for higher cold-neutron intensities to allow, for example, highly sensitive difference measurements by SANS to probe polymer-surfactant interactions

related to tertiary oil recovery and other industrial applications. More-sensitive instruments would also be essential for the study of interfacial behavior of polymer membranes that have potential for future materials separation and electronic applications.

MATERIALS SCIENCE

There are major opportunities in materials-science applications if higher fluxes, along with diffractometers and SANS instruments using enhanced area detection and focusing collimation systems become available. The resulting 1 to 2 orders-of-magnitude increased sensitivity and resolution will greatly extend the size range and level of microstructural features that can be studied in bulk materials. Important advances can be made in the study of nucleation phenomena if the volume fraction of scatterers that can be detected is substantially lowered. Major improvements in neutron facilities will also permit the kinetics of processes such as precipitation, phase decomposition, coarsening, and damage accumulation to be followed in real time (~0.1 to 100 sec). Moreover, complex stress states in metals and composites can be measured with greater resolution. If much larger intensities of very-long-wavelength neutrons become available, the recent extension of SANS diffraction theory to include refraction effects could open up small-angle scattering studies of many materials phenomena that are too large to be described adequately by diffraction alone. These advanced capabilities for microstructure research and evaluation will provide important fundamental information directly related to the

processing, behavior, and reliability of advanced structural materials.

NEUTRON OPTICS

There is considerable motivation to develop much larger perfect crystal interferometers having dimensions of a meter or more, with independently oriented and positioned beam splitters. With these devices one could seriously pursue a neutron Cavendish experiment, higher-order gravitationally induced phase shifts, and a neutron version of the Michelson-Morley experiment. Research involving long-wavelength and ultra-cold neutrons, such as an improved electron dipole moment (EDM) search, will require the development of cold sources with large beams and high fluxes.

Role of Pulsed Sources

While many of the opportunities outlined above can also be addressed in a complementary way by spallation neutron sources (most particularly in neutron-diffraction applications), these sources are new, and we are just beginning to learn how to use both their spectral and pulsed characteristics. The current favorable position of U.S. pulsed-neutron research provides an ideal opportunity to develop these characteristics over the next few years. We already know that pulsed sources are superbly matched to research in both high-resolution and low-resolution diffraction from powders, glasses, and liquids. They exceed reactor sources for applications requiring high-Q or extreme (e.g., high-pressure) environments. In

addition, it is clear that time-of-flight spectroscopy above the thermal neutron range will rapidly become the province of these sources, as improved instruments and higher peak intensities are achieved. However, competitive application of pulsed sources to subthermal neutron-scattering research and to studies of the dynamics of ordered or single-crystal specimens will require the development of new-generation sources and instrumentation. The effective use of cold and "cool" moderators in pulsed sources is an important area, which must be explored further.

For the present, the biggest challenge for spallation sources is how to exploit their rich epithermal spectrum. For example, recent measurements of spin waves up to 150 meV from iron using single crystals, and of electronic crystal-field transitions up to 250 meV in oxide systems, indicate the opportunities in certain applications (magnetic systems, metal hydrides) for the study of high-energy excitations. Similarly, recent incoherent-neutron-scattering studies of high-energy modes in hydrogen-bonded systems show the potential for important neutron spectroscopic applications where optical methods cannot provide needed information on the dynamics of chemical systems. Ultimately, the use of the pulsed structure of these sources by a sequenced application of a variety of stimuli to the sample could open up new applications of neutron scattering.

In sum, pulsed sources open up an extended region, of (Q,) space, and within the next few years we can expect new aspects of condensed matter to be found that lie in this regime. This has been the lesson of neutron scattering for the last 30 years, and we see no reason to change this optimistic view.

Concluding Remarks

One of the clear conclusions that emerges from the recent rapid advances in neutron-scattering instrumentation and sources abroad, and from the more modest developments in the United States over the past few years, is that there is a much broader community, covering many disciplines, that needs and will respond to new and modernized capabilities in neutron-scattering research. Thus, it seems clear that the provision of a new generation of neutron instruments outlined above would more than double the existing neutron-scattering user community, particularly if instrument development is combined with incremental personnel resources to allow a more effective effort for the assistance of users. The role of workshops for the user community and effective user policies and procedures for neutron facilities will also be essential. In fact, it is our view that the increasing importance of neutron-scattering facilities to a broad range of disciplines and users requires the active participation of representatives from these diverse fields in the planning of new instrumentation and sources. Moreover, in order to assure that future neutron sources meet the total needs of U.S. science and technology, it is essential that the university, industrial, defense, and federal laboratory communities have a direct role in establishing the appropriate balance of capabilities to be included in such new sources. It seems most appropriate that an independent, broadly based advisory group should be established by the National Academy of Sciences to provide guidance to the government on the technical characteristics, user policies, and siting of future major neutron centers.

Our examination of existing U.S. neutron sources suggests that a program to allow the United States to achieve an internationally competitive position with other industrialized nations in neutron-scattering research would require an increase from all funding sources of an average of ~$15 million/year (in fiscal year 1983 dollars) capital expenditure over a 5-year period. This would allow, e.g., the timely development or modernization of ~30 critical instruments, including associated cold-source and experimental-hall construction, to meet the new multidisciplinary science opportunities outlined above. A gradual rise in personnel and experimental support to a total increase of ~$12 million at the end of this development phase would be required to allow the science to be done and provide incremental resources for the assistance of hundreds of additional users. Such an investment can be compared with the ~$300 million capital investment in Western Europe during the past decade and the current >$50 million difference in scientific operating expenses between the United States and Europe.

Finally, we would address both the need and the opportunity to plan for a new generation of neutron sources for the mid-1990s and beyond. While current U.S. steady-state sources are and will remain competitive for at least the next decade in innate intensity (if not flexibility), these sources will be between 20 and 25 years old in 1990. We must consider ways in which their capabilities can be replaced with even greater capabilities to meet future scientific needs. Currently, new designs are under consideration for an advanced research reactor featuring increases in power density and total power, which would produce a steady-state flux of about 5×10^{15} neutrons/cm^2-sec. With improved beam-tube design in such

a new reactor, it would be possible to increase neutrons at the sample position for many experiments by an order of magnitude over present generation reactors. Moreover, one advantage of a vigorous testing of pulsed sources and related instrumentation is that new accelerator advances may allow the achievement within the next 15 years of pulsed sources with peak thermal fluxes of ~10^{17} neutrons/cm^2-sec and average fluxes above 10^{14} neutrons/cm^2-sec. For example, design studies have recently been initiated for a next-generation pulsed source based on a fixed-field alternating-gradient (FFAG) proton accelerator. If successful, such a source could ultimately achieve these flux characteristics at a lower capital and operating cost than that projected using current accelerator designs. Thus, there is an immediate opportunity to carry out systematic planning and design for new sources that will clearly be needed by the mid-1990s. Considering the long lead time for the construction and instrumentation of these sources, it is essential that support be provided so that such design efforts may be implemented quickly.

APPENDIX A

INSTITUTIONAL SPONSORS OF USERS OF MAJOR NEUTRON-SCATTERING FACILITIES IN THE UNITED STATES (JULY 1982-JUNE 1983)

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Alfred University	University of Arkansas
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Argonne National Laboratory	National Institutes of Health
Army Armanent Research and Development Command	Naval Research Laboratory
	Naval Surface Weapons Center
Brookhaven National Laboratory	Oak Ridge National Laboratory
Lawrence Berkeley Laboratory	Sandia National Laboratory
Los Alamos National Laboratory	U.S. Geological Survey

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Atomic Energy Agency of Denmark	Kyoto University, Japan
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Chalmers Institute of Technology (Sweden)	Medical Biological Institute of Cambridge, United Kingdom
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CSIRO, Australia	Monash University, Australia
ETH, Switzerland	New South Wales Institute of Technology, Australia
Imperial College, London	
Institut Laue-Langevin	Nuclear Research Institute, Poland
Instituto di Fisica “G. Marconi”	Rutherford Appleton Laboratory, United Kingdom
IVIC, Venezuela	
Japan Atomic Energy Research Institute	Schumber Cambridge Research, United Kingdom
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KFK, West Germany	Technical University of Vienna, Austria
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