# Neutron Scattering: Progress and Prospects

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Over the last decade the unique properties of neutrons have proven useful in a growing number of scientific disciplines. Neutron scattering, traditionally the probe of choice for many magnetic and spectroscopic studies, is now firmly established as an invaluable complement to x-ray scattering for structural and dynamic studies within many other areas of the material sciences, chemistry, and biology. In recent years the instruments and techniques have matured to the point where they are of increasing relevance to the understanding and design of improved practical, everyday materials.

There MAY COME A TIME WHEN OUR GROWING UNDERstanding of exotic elementary particles will allow us to design probes of condensed matter in the way that we manipulate the properties of molecules and genes today. But even with unlimited possibilities, it is hard to imagine improving much on the particle that James Chadwick discovered in 1932. Unlike beams of electromagnetic radiation, electrons, or other charged particles, which interact with matter through long-range Coulomb fields, neutrons interact primarily through nuclear forces and provide an entirely new window through which to observe condensed matter.

Thermal neutrons penetrate deeply into most materials, whereas electrons and (to a lesser extent) x-rays of comparable wavelength are confined to the surface. As a consequence of their relatively heavy mass, neutrons have both energies and wavelengths that match well with the thermally excited states of solids and liquids. By contrast, x-rays and electrons with such wavelengths are much more energetic and so they are unsuitable for studying low-energy excitations and are more damaging to the materials under study. Because of its magnetic moment, the neutron can be used to examine the degree and nature of magnetic order in materials. These properties of the neutron account for the interest in producing beams of neutrons which were used in solid-state physics and chemistry research through the mid-1970s. Since that time, the worldwide growth in the use of neutron scattering has increased both in the number of users and in the number of scientific disciplines involved. Particularly significant for the present and future growth of the field is the growing realization among designers of modern materials (alloys, composites, plastics, adhesives, detergents, and so on) that these materials have reached a degree of sophistication where hit-or-miss, shake-and-bake approaches are ineffective. Fortunately, neutron scattering techniques have now progressed to the point where they can be used in the design of new and improved materials of immediate and direct value to society.

This article surveys some recent examples of the diverse uses of modern neutron scattering. It attempts to update previous reviews of this rapidly evolving field (1). Emphasis is on new techniques such as specular reflectivity in the study of interfacial phenomena as well as on established techniques used to study new materials as diverse as high-temperature superconductors and jet turbine blades. The article concludes with a brief description of the status of U.S. neutron scattering facilities and of plans to regain the initiative in the field that presently resides in Western Europe.

## Surfaces and Interfaces

In recent years, growth in the use of diffraction techniques to study the structural properties of surfaces and interfaces has been exceptional. The large penetration depth of neutrons would seem to make them ill-suited for this purpose, but the unsystematic way in which the neutron cross sections vary across the periodic table and among isotopes of the same element and their strong sensitivity to magnetic moments confer some unique advantages on their use. Presently attainable neutron-beam fluxes, although much weaker than fluxes for synchrotron x-ray sources, are sufficiently strong to permit a variety of experiments that complement x-ray and electrondiffraction studies of surfaces and interfaces. An advantage of using neutrons for such measurements is their ability to penetrate macroscopic distances through substrate materials with little loss, to probe a buried interface.

The principal technique for neutron surface and interfacial studies is specular reflectivity. Just as in classical optics, a beam of neutrons, encountering an ideally flat boundary with a less optically dense medium, will be totally reflected if the angle of incidence is less than a critical angle,  $\theta_c$ , where  $\cos\theta_c = n_1/n_0$ , the ratio of the neutron refractive indices of the two media. The refractive index for most media is less than unity, (1 - n) being typically of the order of  $10^{-6}$ (but dependent on the neutron wavelength and, of course, the neutron scattering density of the material). As a result, total reflection occurs only for very shallow glancing angles less than a few milliradians. For incident angles greater then  $\theta_c$ , the specular reflectivity from an ideally flat interface obeys the Fresnel relation, falling off rapidly [as  $(\theta/\theta_c)^4$  for  $\theta/\theta_c >>1$ ]. Surface or interfacial imperfections (in the form of a graded or rough interface, a third interfacial film, and so on) manifest themselves as deviations from Fresnel behavior. From these measurements, various more or less direct techniques are used to deduce the local interfacial density profile normal to the interface, n(r). The experimentally determined n(r) can then be compared with physically plausible models of the interface (2, 3). The recent advent of dedicated surface reflection

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spectrometers at several neutron scattering faculties in the United States and Western Europe has led to the rapid growth in the application of this technique to problems of surface chemistry, materials and polymer science, and magnetism that parallels the widespread interest in small-angle neutron scattering (SANS) that developed a decade earlier.

Studies have been carried out on the interfacial profile between a liquid and its saturated vapor (4), adsorption of surfactants (2) and polymers (5) at the air-solution interface, liquid-solid interfaces (6), the structure and drainage of black soap films (7), and Langmuir-Blodgett (4) multilayer films. A typical neutron scattering "trick" that can be played when studying the air-water interface is to use an 8.8 mol-% D<sub>2</sub>O-H<sub>2</sub>O mixture, which produces null reflecting (n = 1) water. Thus, apart from diffuse background scattering, which is easily subtracted, there is no signal at all from either the air or the water substrate, and the reflection results entirely from the adsorbed surface layer. Isotropic substitution can be further used to highlight particular parts of the adsorbate molecules, as in SANS (8).

Taking advantage of the large specific surface area of materials such as exfoliated graphite and MgO "smoke," researchers using conventional elastic and inelastic neutron scattering techniques have contributed greatly to the present understanding of layering and wetting phenomena and surface melting of physisorbed molecules (rare gases, light hydrocarbons) on these substrates (9). For example, elastic and quasi-elastic neutron scattering studies of the melting of submonolayer ethylene films on graphite show evidence for a continuous melting transition, as predicted by the dislocation-pair unbinding theory of two-dimensional melting (10).

## Polymers

Conventional light and x-ray scattering experiments provide easily understandable information about polymers only in dilute solutions. Consequently, much of the present detailed understanding of the molecular conformation of semidilute, concentrated, and bulk polymers has come from the same conjunction of selective deuteration, contrast variation, and SANS investigations that has proven so incisive in the study of biological structures. Scaling concepts, in part tested by earlier neutron studies of fluid and magnetic systems, have proved relevant to a deeper understanding of polymer physics as well (11). SANS studies have demonstrated that, at short distances, concentrated polymers retain the self-avoiding random walk geometry characteristic of isolated polymers but that, at larger distances, polymer-polymer interactions cause the random walk to lose its self-avoiding character (12).

The "alloying" of polymer blends offers a means to control the structure and properties of polymeric materials at various spatial and compositional levels. This knowledge can be put to a variety of practical uses, particularly in problems of polymer compatibility encountered in the recycling of plastic wastes (1). Quantitative understanding of the thermodynamic properties of polymer blends (mixtures of two or more polymers) has traditionally come by way of the application of approximate mean-field theories to "neutron cloud point" studies (13). In recent years, SANS studies have helped define the limits of applicability of this approximation with studies of crossover from mean-field to non-mean-field (Ising) behavior in model systems (14). Even binary mixtures of protonated and deuterated polybutadiene with a sufficiently high degree of polymerization have been shown to phase-separate at low temperatures, contradicting the widely held belief that such mixtures form ideal solid solutions (15).

Polymerization of two distinct monomer types (such as styrene and isoprene) gives rise to materials known as block copolymers, which are finding increasing use as surfactants, emulsifiers, and adhesives in biomedical and microelectronic applications. At sufficiently high temperatures bulk copolymers exist as an isotropic disordered phase, whereas various ordered structures (for example, lamellar, hexagonal, or cubic) arise at low temperatures. Their structure, morphology, and phase behavior are of both practical and fundamental interest. A recent neutron scattering study of the order-disorder phase transformation in one such system has demonstrated non-mean-field critical scattering over a surprising large temperature range (60 K) above a fluctuation-induced first-order transformation temperature (16).

Neutron specular reflectivity techniques have also been applied to polymer studies. Surface-induced phase separation of symmetric block copolymer films has been observed on various substrates. Examples of the quality of the data and fits to determine the normal scattering density profile are shown in Fig. 1. Interfacial widths accurate to better than 10% are obtained, but the values are not well described by current theories (17).

By the use of an elegant new high-resolution inelastic scattering technique, neutron spin-echo spectroscopy (18), neutrons have begun to provide microscopic information on polymer elasticity and rheology. In an idealized picture of low-frequency polymer-chain dynamics, a diffusing chain segment of length  $\sigma$  performs a random walk in a space defined by all possible spatial chain configurations. In this so-called Rouse model, the time-dependent neutron scattering function, S(Q,t), where Q is momentum transfer and t is time, which contains only one characteristic distance,  $\sigma$ , obeys a predictable scaling behavior. S(Q,t) has been measured for several polymer systems and shown to obey Rouse scaling at short times t. Deviations from Rouse scaling have been observed at longer times (19). The deviations can be explained by introduction of an additional dynamic length scale, intermediate between segment length and the end-to-end chain length, specifying an entanglement distance not considered in the Rouse model. The appearance of this new length scale confirms an essential assumption of the reptation theory of polymer viscoelasticity developed by deGennes (11).



**Fig. 1.** Neutron specular reflectivity R versus scattering angle for thin annealed films of diblock copolymers on a Si substrate, which induces phase separation of the two polymer constituents. The inset shows the scattering density profile that was deduced on the basis of a fit to the data;  $k_{oo}$  momentum; b/V, impact parameter per unit volume; z, distance (17). [Reproduced from (17) with permission of the American Institute of Physics]

## Biology

Neutron scattering plays two different roles in biological research, both arising from the special properties of hydrogen. At high resolution, neutrons are used in conjunction with electron density maps established by x-ray studies, and in which hydrogen atoms are not visible, to complete the structure determination. At lower resolution, SANS experiments utilize the different scattering power of hydrogen and deuterium to selectively reveal particular aspects of complex biological assemblies (20).

Water-soluble proteins are known to be surrounded by rather loosely bound shells of water molecules. In protein crystallography it has been customary, until recently, to ignore this water of hydration in refinement procedures. This is technically possible because the water molecules are sufficiently delocalized and disordered to make their presence felt only in low-order diffraction peaks. In order to improve the description of the surface structure of proteins, new methods of analysis have been developed that include water of hydration in a tractable manner, allowing all of the diffraction peaks to be used in the refinement. Figure 2 shows the surface structure of carboxymyoglobin derived in this way (21). All of the bound water molecules are associated with polar or charged groups on the skeletal surface of the protein.

The functions of biologically active species such as proteins are strongly influenced by the overall conformation (tertiary structure) of complex structures as well as by the details of the amino acid sequences. One can obtain such information through small angle scattering studies, methods familiar in the study of dilute polymer solutions. Plasminogen, a single chain polypeptide containing 790 amino acids, which when activated to plasmin catalyzes the dissolution of blood clots, is an example. Recent SANS studies have shown that the occupation of a bonding site for the amino acid



**Fig. 2.** A skeletal model of the respiratory protein carboxymyoglobin. The oxygen-binding heme group is in purple, the main amino acid chain in blue, with acidic and basic side chains in orange and green, respectively. Recent neutron scattering results have allowed the determination of the position of 87 weakly bound surface water sites indicated by space-filling dotted clusters. Access to the heme site is not blocked by the surface water (21). [Reproduced from (21) with permission of the International Union of Crystallog-raphy]

lysine in native human plasminogen produces a more easily activatable form in which the radius of gyration changes from 39 to 56 Å (22). More detailed information about the conformation is contained in the length correlation function, P(r), shown in Fig. 3. [P(r), which gives the probability that two atoms separated by distance r are in the same particle, can be derived from the SANS data by Fourier transformation.] These probability distributions suggest that the less active, closed form adopts a shape of a prolate ellipsoid of revolution, whereas the active, open form is that of an extended flexible coil.

At the next level of structural complexity, one encounters functional entities such as ribosomes, which translate the genetic code into specific sequences of amino acids to produce proteins. Because ribosomes have not been prepared in crystalline form, the conventional crystallographic approach is not useful. However, by selective deuteration a low-resolution, three-dimensional reconstruction of the constituent proteins based on triangulation can be inferred. All ribosomes can be separated into two unequal subunits. For the bacterium *Escherichia coli*, where the necessary preparation of deuterated proteins can be carried out in heavy-water culture media, the smaller subunit, known as 30S, contains 21 different proteins. A total of 79 individual SANS experiments, spread over many years, has succeeded in mapping the relative positions and radii of gyration of 15 of the 21 proteins (23). Similar studies on the larger subunit are also in progress (24).

Viruses, which typically consist of a protein coat enveloping a genetic DNA or RNA, are also well suited for study by neutron contrast variation. In large animal viruses, such as the influenza or the common cold virus, the distribution of the various components is otherwise practically impossible to determine. For example, neutron contrast variation has recently been applied to a single crystal of tomato bushy stunt virus, showing that the protein is distributed in two shells, the outer capsid (whose structure was known from x-ray studies) and an inner, less well-ordered shell (20). In nucleosomes, the basic subunit of chromosomes, contrast matching has been used to establish that the DNA is wrapped around the protein rather than vice versa (1).

New information concerning the regulation of protein synthesis in living bacterial cells has been obtained in a recent study of the so-called *tet* gene. This gene is responsible for the production of a



Fig. 3. Changes in the length distribution function (see text) for the human blood-clotting agent plasminogen, associated with a ligand-induced change in the folding of the macromolecule. The closed form (solid line) is an ellipsoid of revolution; the more active, open form (dashed line) is an extended flexible coil (22). [Reproduced from (22) with permission of the American Association for the Advancement of Science]

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protein in host bacteria that makes them immune to the antibiotic tetracycline. The production of proteins can be switched off by binding other repressor protein molecules to specific regions of the bacterial DNA molecule. SANS studies have determined both the position and the conformation of a repressor protein for the *tet* gene, showing that the repressor provides a geometrical obstacle to the active part of the gene (25).

A promising new method for the alignment of macromolecules in SANS experiments, which eliminates the loss of structural information due to orientational averaging of the molecular form factor, has been demonstrated. Ferrofluids, stable aqueous suspensions of small (100 Å) paramagnetic particles, when magnetized to saturation in an external field (on the order of 0.5 T), develop a preferential alignment that can be transferred by cross correlation to codispersed nonmagnetic particles, which act as magnetic holes. Dilute dispersions of rod-shaped tobacco mosaic virus and tobacco rattle virus have been ordered into nematic-like structures in this manner, under conditions in which pure dilute suspensions cannot be ordered by conventional means (26).

To date, little has been done in the area of diffuse and inelastic scattering of biologically interesting molecules, although the increasing availability of large amounts of genetically engineered samples suggests that this situation will soon change. One notable example is the study of wet-spun DNA fibers, which exhibit strong hydration-dependent planar sheets of diffuse scattering normal to the axis of the helix. These features can be interpreted as arising from water molecules whose positions are strongly correlated only along the DNA chains but whose period is incommensurate with the DNA repeat distance. The scattering appears to be entirely inelastic, consistent with what would be expected from a quasi–one-dimensional liquid (27).

### Neutron Powder Diffraction

For many materials neutron diffraction offers decisive advantages over other techniques for structure determination at the atomic level. This is particularly true for materials for which single-crystal specimens are not available. Steady advances in instrumentation and data analysis, combined with the unique properties of the neutrons themselves, now make it possible to obtain structural precision with powder neutron techniques comparable in many cases to that obtainable by single-crystal methods.

Unlike x-rays or electrons, which scatter preferentially from elements with high atomic number, neutrons are capable of accurately locating light elements (such as hydrogen, lithium, carbon, nitrogen, and oxygen) even in the presence of much heavier ones. Intractable site occupancy problems involving atoms with similar x-ray scattering power [as, for example, in industrially important Al-Si zeolites (28)], can be readily solved with neutrons. Because neutrons are much less absorbing than electrons or x-rays of comparable wavelength, it is straightforward to perform experiments in special sample environments (cryostats, pressure cells, furnaces) (29). Typical sample sizes range from 1 to 10 g, but successful experiments have been performed on samples of less than 50 mg.

A major factor contributing to the popularity and success of neutron powder diffraction is the Reitveld data analysis method (30), in which computer fitting of pattern linewidths is used to extract intensities of overlapping peaks. This method is primarily a technique for refining the structural parameters of an approximately known structure. Refinements of about 100 parameters (structures with 20 to 30 crystallographically distinct atomic sites) can be routinely carried out at the present time. However, a partial or approximate initial structure is not always necessary. Progress is being made in applying direct (31), Patterson (32), and Monte Carlo (33) methods to ab initio powder neutron structure determinations.

The capability of neutron powder methods has proven decisively important in sorting out the nature and role of oxygen defects and disorder in high-temperature superconductors. The best studied of these new materials to date is the 90 K superconductor YBa2Cu3O7-x. This relatively complex oxide structure normally has a large number of oxygen defects ( $x \approx 1$ ), and the superconducting properties depend strongly on both the concentration and the ordering of these oxygen defects. The filling of the available oxygen sites, including high-temperature studies in controlled oxygen atmospheres, has been extensively studied by neutron powder diffraction (34). There are two kinds of Cu sites in the structure: Cu(1) layers, forming one-dimensional Cu-O chains, and Cu(2) layers, in the form of CuO<sub>2</sub> planes. It is believed that the superconductivity occurs in the CuO2 planes, which are doped by holes transferred from the Cu-O chains, which act as charge reservoirs. The variation of the superconducting transition temperature  $T_c$  with x is striking, with a 90 K plateau near x = 0 and a 60 K plateau centered near x= 0.5, whose existence and extent seem strongly correlated to the degree of ordering of the oxygen defects as well as their concentration. Superconductivity is completely suppressed above x = 0.65. A combination of neutron and anomalous x-ray powder diffraction has been used to determine the site-specific valence of the Cu ion in the plane and chain sites in YBa2Cu3O7-x, as well as the site preference for other cationic dopants in this material (35). This is an outstanding example of the powerful complementarity of x-ray and neutron scattering techniques.

The ability to reliably measure the distribution of residual stress fields-elastic stress fields that exist in the absence of external forces and that are created through the differential action of plastic flow or thermal contraction-is vital to the safe and efficient design of modern composite materials, fabrications, and weldments. Neutron scattering provides the only nondestructive technique for measuring the absolute stress tensor in a bulk specimen. The principle, which is identical to that in which x-rays are used, is to determine the local internal stress through the measured elastic lattice strain that it produces. One determines the strain from the shift of the lattice plane spacing d, using Bragg's law, and, because the strains are small (typically  $\Delta d/d = 10^{-4}$ ), extremely good instrumental resolution is required. The volume of the sampled region is defined by the overlap of the paths of the incident and diffracted beams, so the best spatial resolution occurs when the beam is diffracted at a right angle (36). Recent residual stress studies have, for example, been directed toward understanding of fatigue in utilitarian objects such as railway rails, welds in oil pipelines, and heat exchangers for nuclear reactors (37), as well as toward improving the properties of SiC-reinforced aluminum alloys and WC-based cemented carbide composites (38). Neutron diffraction is also used to determine bulk preferred orientation, or texture, in polycrystalline samples, including such materials as jet engine turbine blades, where crystalline grain orientation is used to enhance strength and performance (1).

## Magnetism

The continuing importance of neutron magnetic structure determination is well demonstrated by studies of high-temperature superconductors. In the undoped, insulating prototypes of the superconductors, the  $CuO_2$  layers exhibit strong two-dimensional antiferromagnetic correlations and may exhibit three-dimensional long-range order that persists to elevated temperatures. Doping the  $CuO_2$  planes with either holes or electrons transforms these materials from antiferromagnetic insulators to metallic superconductors.



**Fig. 4.** In high- $T_c$  superconductors such as  $La_{2-x}Sr_xCuO_4$ , antiferromagnetic correlations persist upon doping into superconducting region of the phase diagram (x > 0.07), suggesting that the superconductivity may be mediated by exchange of spin excitations. The line represents the average distance between holes introduced by Sr doping (41). [Reproduced from (41) with permission of the American Institute of Physics]

In these insulators, studies of the value of the ordered moment, its temperature dependence, and the magnetic form factor are consistent with localized Cu spins with strong Heisenberg coupling between nearest in-plane neighbors and very weak interplanar coupling (39). The strong intraplanar coupling has also been verified by direct measurement of the spin-wave velocity by inelastic scattering (40). Neutron studies reveal that long-range antiferromagnetic order disappears quickly with doping. Because of the large in-plane coupling, substantial two-dimensional short-range correlations per-

sist even in the metallic superconductors (41) (Fig. 4). Their existence gives plausibility to theories that ascribe the superconducting pairing interaction to virtual spin-wave exchange rather than the phonon mechanism of conventional superconductors (42). The relation between superconductivity and spin fluctuations has also been a topic of intense interest in the so-called heavy-electron superconductors such as UBe<sub>13</sub>, UPt<sub>3</sub>, and URu<sub>2</sub>Si<sub>2</sub>, because neutron scattering measurements reveal that antiferromagnetic order and, in some cases (43), propagating spin waves coexist with the superconductivity.

Extensive studies of synthetic multilayer films have been motivated by both scientific and practical concerns, because such films serve as mirrors and monochromators for neutrons and x-rays (44). Polarized neutron diffraction has been used to study magnetic multilayers, to determine the effect of reduced dimensionality in thin magnetic films (45). Studies of single-crystal multilayer superlattices consisting of rare earth layers alternating with yttrium reveal long-range magnetic order that is propagated through intervening nonmagnetic yttrium layers. In the case of Dy, the phase and chirality of the helical order are preserved from one Dy layer to the next. The phase shift across the yttrium layer is proportional to its thickness, suggesting that the coupling is propagated by a spin-density-wave (RKKY) mechanism (46).

Sputtered films of ferromagnetic  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> are promising materials for use as high-density magnetic recording materials. The thicknesses of these films (fractions of micrometers) make conventional probes for magnetic depth-profiling inadequate. (For example, spin-polarized photoemission is sensitive to only the topmost atomic layers.) When combined with the use of polarized neutrons, specular reflection techniques are well suited to these measurements and reveal the presence of a 150 Å thick magnetically dead layer at the surface of the film. Similarly prepared Fe<sub>3</sub>O<sub>4</sub> films, which are inferior for recording purposes, show no such magnetic dead layer (47).

It has been shown that by capping a thin ferromagnetic film with an appropriate nonmagnetic overlayer a significant enhance-





ment (50 to 100) of the spin-dependent reflectivity can be obtained (48). This technique has been used in a series of measurements of magnetization and anisotropy of thin (20 Å) epitaxial layers of Co and Fe on (100) Cu substrates (49). Polarized neutron reflectometry has also been used to measure the magnetic flux penetration depth in type II superconductors (50).

The unique characteristics of neutrons are used in a novel way in the study of nuclear magnetism-the long-range ordering of nuclear spins that occurs in some crystals at very low temperatures. The sensitivity of the neutron to the nuclear spin order arises because a spin-polarized nucleus exhibits a different scattering cross section for spin-up and spin-down neutrons. In a recent experimental tour de force, the magnetic phase diagram of a single crystal of <sup>65</sup>Cu in an external magnetic field was determined. At temperatures below a Neel temperature T<sub>n</sub> of 58 nK, three distinct antiferromagnetic phases, separated by two first-order phase transformations, have been identified. In these measurements, the sample, which could be held below the Neel temperature for about 5 min at a time, was repeatedly cooled by adiabatic demagnetization in a 36-hour cycle. At the highest fields a new commensurate magnetic structure, unknown in any conventional face-centered cubic antiferromagnet, was found (51).

### Neutron Spectroscopy

The examples discussed so far have involved primarily elastic neutron scattering. Because cross sections for inelastic scattering are invariably much smaller than for elastic scattering, great care has gone into designing specialized neutron instruments optimized for a particular compromise between resolution (momentum as well as energy) and intensity. Instruments now exist that provide coverage of six to eight orders of magnitude in both energy and momentum (wavelength). Figure 5 shows some of the types of processes that are being investigated by present-day inelastic scattering techniques (52).

The classical triple-axis techniques for phonon and magnon studies have progressed to the point where much more complex structures can be analyzed. Significant recent examples include high-temperature superconductors. Nearly complete energy-momentum relations exist for La<sub>2</sub>CuO<sub>4</sub> (53), for which a soft phonon mode causes structural phase transformations (54) [which can, in turn, influence the superconductivity (55)]. Phonon density-of-states measurements have been made for many of the copper oxide superconductors (53), although the role of phonons in the electron pairing mechanism is still uncertain. Studies of the lattice dynamics of hydrogen-, deuterium- and tritium-substituted PdH have clarified the cause of the reverse isotope effect on the  $T_c$  values of these materials (56).

The availability of epithermal neutrons from reliably operating pulsed spallation sources has dramatically increased the use of deep inelastic scattering (energy transfer, 100 to 1000 meV). The atomic potentials of hydrogen dissolved in metals have been probed by studies of anharmonic shifts in the higher state vibrational energies. A different deep inelastic scattering technique, neutron Compton scattering, has been used to measure the momentum distribution of hydrogen in metals (57), as well as liquid and solid hydrogen and helium (58). These data can in principle also be transformed into information on the atomic potential (59). Intermultiplet electronic transitions with weak or forbidden optical selection rules have been studied by inelastic neutron scattering in rare earth and actinide compounds at energies exceeding 1 eV. For example, the presence of such well-defined transitions in the heavy-electron superconductor UPt<sub>3</sub> establishes that hybridization does not completely destroy the



**Fig. 6.** (**A**) Ground-state tunneling splitting due to rotational tunneling in deuterated nitromethane, determined by back-reflection spectroscopy;  $\Delta \epsilon$ , energy difference. (**B**) The rotational potential function deduced from such measurements, showing the energy levels for hydrogen- and deuterium-substituted molecules (61). [Reproduced from (61) with permission of the American Institute of Physics]

localized atomic nature of the atomic states in this material (60).

Similar gains have been made in the microelectron volt range of the spectrum. There is now a well-defined subfield of molecular chemistry devoted to the study of rotational modes of molecules in solids. Driven by the availability of high-resolution back-reflection spectrometers situated at high-performance cold neutron moderators, these studies are providing information on intermolecular potentials previously inaccessible to spectroscopic study. Figure 6 shows an example of rotational tunneling spectra in nitromethane, together with the rotational potential deduced from a comparison of these and other higher energy neutron measurements (*61*). The spin echo spectrometer, useful for polymer studies, is capable of resolving diffusive motions down to the 10-neV energy scale (*62*).

Time-of-flight inelastic scattering techniques, which measure the scattering from many excitations simultaneously, are well suited to the study of the structural network dynamics of glasses (63). A major puzzle in recent years concerns the nature of excess low-frequency excitations in glasses, which contribute anomalously to their heat capacities and acoustic attenuation. Figure 7 shows the frequency distribution of excess modes in vitreous silica derived from inelastic neutron scattering measurements. The variation of scattering intensity with scattering angle is consistent with that expected from rotations of corner-coupled SiO<sub>4</sub> tetrahedra. Above 0.5 THz (2 meV) the modes appear to be harmonic, but at lower frequencies they are described by an anharmonic relaxational behavior. The results have been used to develop a common framework for understanding the thermal, acoustic, and optical anomalies in vitreous silica (64).

Recently, a combination of neutron and Raman scattering spectroscopies has been used to investigate the density of vibrational states of tenuous, fractal materials. If the material is fractal below a certain correlation length,  $\xi$ , and homogeneous on a longer scale, one expects conventional phonon-like behavior for vibrations with wavelengths greater than  $\xi$  and a different, "fracton"-like, behavior for wavelengths smaller than  $\xi$ . Such qualitative changes in behavior have been observed in fractal silica aerogels (65). Inelastic neutron scattering studies have also shown that well-defined, isotropic acoustic phonon modes (both transverse and longitudinal) exist in icosahedral, so-called "quasi-crystalline" AlCuFe ternary alloys in spite of their lack of long-range translational symmetry (66).

## Current and Future U.S. Prospects

Although they have not kept pace with developments in Western Europe, improvements in U.S. neutron scattering facilities are ongoing. The experimental hall at the Los Alamos Neutron Scattering Center (LANSCE) has been expanded to accommodate new instruments, and a more efficient enriched uranium target has been recently installed at the Intense Pulsed Neutron Source (IPNS). A new guide hall is in advanced state of construction at the National Institute of Standards and Technology reactor. When fully completed in 1993, it will provide about 15 new experimental stations and new capabilities (such as spin-polarized inelastic scattering and back-reflection inelastic scattering) for use by U.S. scientists. Plans exist for a similar extension of the capabilities of the High-Flux Beam Reactor (HFBR) at Brookhaven and the High-Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory.

In spite of the steadily growing interest in neutron scattering by scientists in many disciplines and the gradual advances in the capabilities of facilities, the health of U.S. neutron scattering cannot be described as robust. In the wake of well-publicized safety and environmental concerns at defense-related Department of Energy facilities, both HFIR and HFBR have recently been subjected to abrupt and extended shutdowns for safety reviews. The damage from the resulting "neutron drought" extends beyond the inevitable lost scientific opportunities. These unanticipated disruptions have caused many scientists whose research grants and careers are based on predictable access to neutrons to question the wisdom of such commitments.

Another cause for concern is the steep rise in the cost of running major facilities (especially reactors), largely driven by security- or safety-related improvements. These costs, often in the form of sudden, high-priority demands ill-suited to the normal budget process, further reduce the funding necessary to operate the facilities at a level approaching optimum efficiency. As a result, both IPNS and LANSCE operate on only a half-time basis, and both HFBR and HFIR have a complement of 25-year-old instruments which, if upgraded to modern standards, would effect cost recovery in terms



Fig. 7. The frequency distribution of low-energy vibrational states in vitreous silica compared with that expected by acoustic phonons. The excess density of states contributes to the anomalous heat capacity (64). [Reproduced from (64) with permission of the American Institute of Physics]

of increased performance within a single year.

The most ambitious and exciting U.S. plans for the future are for an Advanced Neutron Source (ANS), presently being developed at Oak Ridge National Laboratory (1). When completed, the ANS will become the world's highest flux reactor for neutron scattering and will provide state-of-the-art isotope production and materials irradiation facilities as well. The increased flux will make feasible the design of entirely new instruments that do not exist today in the United States or in the world. It will then be possible to perform experiments that are either impossible or impractical at the present time. Examples of such experiments include the routine use of neutron polarization techniques, which permit separation of nuclear and magnetic scattering as well as separation of coherent and incoherent scattering arising from nuclear spins (67). With the appropriate instrumentation, the higher flux can be translated into faster data acquisition to improve the study of time-dependent nonequilibrium phenomena, as well as studies at higher energy and momentum resolution. The ability to study smaller samples is important in many areas, where large samples are impossible to obtain.

With an optimal funding profile, conceptual design of the ANS would be completed in 1992, with construction beginning in late 1994. The earliest anticipated date for completion of construction is the year 2000. With an estimated cost in excess of \$0.5 billion, the ANS will require the same degree of support from the scientific community that has propelled the growth of the synchrotron light sources in this country. With such support, the United States will be assured of a superb focus for neutron scattering activities well into the next century.

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# Diversity of G Proteins in Signal Transduction

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The heterotrimeric guanine nucleotide-binding proteins (G proteins) act as switches that regulate information processing circuits connecting cell surface receptors to a variety of effectors. The G proteins are present in all eukaryotic cells, and they control metabolic, humoral, neural, and developmental functions. More than a hundred different kinds of receptors and many different effectors have been described. The G proteins that coordinate receptor-effector activity are derived from a large gene family. At present, the family is known to contain at least sixteen different genes that encode the alpha subunit of the heterotrimer, four that encode beta subunits, and multiple genes encoding gamma subunits. Specific transient interactions between these components generate the pathways that modulate cellular responses to complex chemical signals.

LL BIOLOGICAL SYSTEMS HAVE THE ABILITY TO PROCESS and respond to enormous amounts of information. Much of this information is provided to individual cells in the form of changes in concentration of hormones, growth factors, neuromodulators, or other molecules. These ligands interact with transmembrane receptors, and this binding event is transduced into an intracellular signal. Several families of cell surface receptors have been characterized that are coupled to different mechanisms of signal transduction. Here, we examine the signal processing mechanisms of receptors that are coupled to G proteins (1).

Signal transducing G proteins occur in two forms, the "small G proteins" that are generally found as single polypeptides composed of about 200 amino acids and the heterotrimeric G proteins that are made up of  $\alpha$ ,  $\beta$ , and  $\gamma$  subunits. The small G proteins function in regulating cell growth, protein secretion, and intracellular vesicle interaction (3). The heterotrimeric G proteins are associated with signal transduction from cell surface receptors (4) and are thought to act as switches that can exist in either of two states depending on bound nucleotide (Fig. 1). A large family of transmembrane receptor proteins that share a characteristic topological structure has been revealed by molecular cloning and biochemical or pharmacological studies. All of these proteins have seven membrane spanning domains and show considerable amino acid sequence similarity (2). Signal transduction by these receptors is initiated by ligand binding which stabilizes an alternate conformational form of the receptor and thus transmits information across the cell membrane. This leads to a complex series of events that we understand only in broad outline. The ligand-bound receptor initiates two processes; one leads to desensitization, and occurs through receptor modification (5), and the other is a signal generating process that begins with the activation of the heterotrimeric G protein (Fig. 1A). Interaction of the G protein with the activated receptor promotes the exchange of guanosine diphosphate (GDP), bound to the  $\alpha$  subunit, for gua-

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