gap has been measured by other spectroscopic techniques, these methods suffer from surface problems, Axe told us. Both tunneling and infrared spectroscopy measure the energy gap at the metal surface, which may differ from the bulk value, Axe said. He feels that although the Brookhaven measurements are not terribly precise, they are clearly bulk measurements. —GBL

Neutrons probe protein structure

Although x-ray diffraction has for years been valuable in revealing the structure of biological molecules, some kinds of information have remained beyond the reach of x rays. More recently, neutron diffraction has been applied in biophysics,[1] and some experimenters at Brookhaven National Laboratory have successfully used neutrons to map such large complexes as sciatic nerve membrane (myelin)[2] as well as for the location of individual hydrogen positions on smaller, more ordered molecules such as the protein myoglobin.[3] Most of the work has been done at the Brookhaven High Flux Reactor with equipment built by Benno Schoenborn of the BNL biology department.

A major drawback for x rays in biological-structure studies is their inability to locate hydrogen atoms. Hydrogen, which plays a significant role in enzyme action, has a very low x-ray scattering factor. (X-ray form factors increase with atomic number.) Neutron-diffraction studies of hydrogen, on the other hand, exploit the dependence of scattering on nuclear size and on nuclear spin. Because hydrogen and its isotope deuterium have scattering factors that differ in sign as well as in magnitude, isotopic substitution can show clearly where the hydrogen atoms are. Similarly, nitrogen (atomic number $Z = 7$, number of nucleons $A = 14$) is distinguishable from carbon ($Z = 6$, $A = 12$) and from oxygen ($Z = 8$, $A = 16$).

Unlike x rays, the neutrons cause no significant radiation damage, so that a single crystal can be used repeatedly—an important advantage, particularly for large, hard-to-grow crystals. The use of one crystal throughout an experiment also eliminates problems caused by differences between crystals. And with neutrons, the problem of phasing (how do you know which diffraction order you are observing) is resolved through the anomalous dispersion of heavy isotopes such as Gd^{157}, Sm^{149} and Cd^{113}.

Neutron fluxes from even the most powerful sources, such as the Brookhaven reactor, are only about 10^{-5} times as great as available x-ray fluxes. This major disadvantage is compensated for with larger crystals (possible because neutron absorption factors are considerably smaller than x-ray absorption factors) and by longer exposure times. Neutrons, being nonionizing, are harder to detect than are x rays. They must be converted to ionizing radiation by reactions with such nuclei as boron and He^3 and then detected.

Myoglobin. Schoenborn has nearly completed a study of myoglobin, a relatively simple protein that can be crystallized. He is aiming at atomic resolution and regards this work as a prototype experiment to assess the feasibility of studying other proteins. He uses the myoglobin structure found by John Kendrew and his colleagues[4] (nonhydrogen atoms only) as a basis for phase determination and has located a majority of the hydrogen and deuterium atoms present, as well as over 100 water molecules clearly associated with polar surface groups on the myoglobin.

The myoglobin experiments were done with a single large crystal (4 mm × 3 mm × 2 mm) that had been soaked in deuterated mother liquor; here D_2O replaced much of the H_2O, reducing the incoherent scattering by hydrogen, which is of course present in both spin-up and spin-down states. A germanium-crystal monochromator selected 1.6-Å neutrons from the high-flux beam, and the resulting neutron flux at the sample is about 10^7 per cm^2 per sec. He measured about 10 000 reflections, with a counting time of five minutes per reflection; the average background was about 100 counts per minute and the strongest signal count about 22 000 per minute.

From the data, hydrogen (or deuterium) bonding between the CO (carbonyl and NH (amide) groups of the various amino acids forming the myoglobin can be determined. These hydrogen bonds are largely responsible for the three-dimensional (helical) order of the myoglobin.

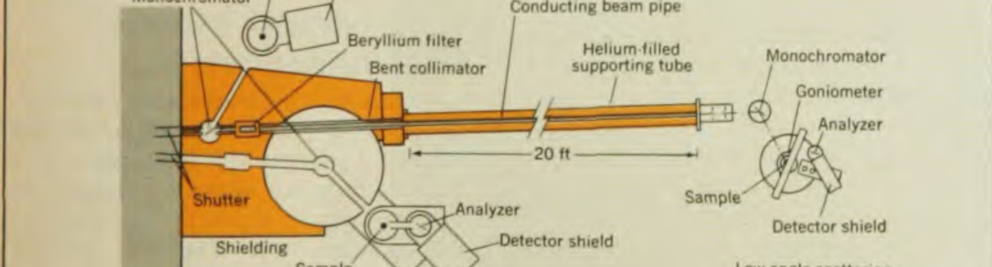
A total of 106 water molecules were located, 8 on the "main chain" amides, 30 on the "main-chain" carbonyls and the remainder on side chains. Different myoglobin molecules were found to be linked by nine water bridges and ten salt bridges.

Schoenborn points out that the results should be treated with caution in this first attempt at detailed protein analysis. Errors are probably present because of inaccurate phase determinations or other effects. Once an anomalous phased neutron map has been completed, he will have a better idea of the validity of the myoglobin results.

Large protein complexes. For a neutron-diffraction study of rabbit sciatic nerve membrane, the spacings involved are rather large (about 200 Å), and Donald Caspar (now at Brandeis), Schoenborn, Anthony Nunes and Donald Kirschner used relatively long-wavelength neutrons to achieve high resolution. The aim here is to determine molecular, rather than atomic, arrangement, with resolution about 10 Å.

Soaking the membranes in a D_2O solution substituted deuterium for part of the exchangeable hydrogen. The beam pipe and a beryllium filter remove all but lower-energy ($\lambda > 4$ Å) neutrons. By comparing the neutron and x-ray results, the chemical identity of some x-ray Fourier peaks were determined.

Donald Engelman and Peter Moore (both at Yale), who also do their experiments with the BNL apparatus, have suggested[5] a novel way to determine the gross (quaternary) structure of the protein complexes known as ribosomes;



Neutron diffraction in biology. Beam from the Brookhaven High Flux Reactor separates into components for the double-axis and beam-pipe spectrometers. A germanium monochromator selects shorter-wavelength neutrons for relatively high-resolution work, such as the myoglobin studies. The beryllium filter and beam pipe provide neutrons with wavelength greater than 4 Å for molecular-arrangement studies of large complexes.

that is, to work out a three-dimensional map of the positions of the 50 or so proteins and the nucleic acids that form the macromolecular ribosome complex. They would take the deuterated form of the ribosome, separate it into its constituent proteins and RNA, hydrogenate two of the proteins, then reassemble the ribosome. Neutron diffraction can then give the distance between the two nondeuterated proteins; repeating the process for all the remaining protein pairs would lead to a three-dimensional map of the structure. The experiments on ribosomes are now in a preliminary stage, and Caspar and Michael Moody plan to use similar methods for other macromolecules.

Improvements. The major limitations to neutron diffraction as a tool in molecular biology now appear to be those of source strength and instrumentation. Among the techniques currently being explored[1] are beam focusing through graphite monochromators, better beam pipes, and a multidetector ("hedgehog") counting system, now being built for the high-flux beam reactor in Grenoble (see PHYSICS TODAY, September 1972, page 17). Alternatively, monochromators could be eliminated and a time-of-flight method used to analyze the pattern produced by the entire neutron spectrum. —MSR

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Metallic hydrogen

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The Livermore group, Ronald S. Hawke, D. E. Duerre, J. G. Huebel, R. N. Keeler and H. Klapper, reported an apparently similar experiment last March at the High Pressure Physics and Planetary Interiors Conference in Houston. They determined that liquid hydrogen had a volume of 1 cm^3/g at a pressure of about 2 megabars but they say they did not determine if it was transformed into a metal. Hawke says that pressure-volume measurements alone (with their associated errors) are not capable of pinning down the metallic transition pressure. "We have a point in the ballpark of the metallic equation of state, but I'm reticent to say that proves it's metallic hydrogen." Livermore hopes in the very near future to have a direct electrical measurement of the hydrogen metal transition; that is, they will measure the electrical conductivity as the sample changes from an insulator to a metal.

There are actually two Livermore programs that are measuring hydrogen's properties at high density. Both are dynamic methods: relatively fast shock compression and relatively slow isentropic compression using a strong magnetic field. The latter method (suggested by Francis Bitter in 1965), which Hawke and his collaborators use, is deliberately made slow enough (about 10 microsec) that no shock waves are generated in the sample.

Hawke and his colleagues use two concentric conducting cylinders that surround a cylinder of liquid hydrogen; the outer cylinder is four inches in diameter and the inner one is 0.5 inches in diameter. The outer cylinder is driven inward with high explosives shortly after a 60-kG magnetic field is applied between the cylinders; the field serves to transfer momentum from the outer to the inner cylinder. Because flux is conserved, as the area of the interior goes down, magnetic-field intensity increases, going up to 10 MG in about 10 microsec. The field squeezes on the smaller cylinder, generating a pressure on the hydrogen sample. The hydrogen compression time is long enough (much longer than in the shock experiments) that sound can traverse the sample several times, so that the compression is isentropic.

The experimenters make a 0.2-microsecond flash x-ray exposure before the experiment and during it. By comparing the sample-tube diameter before and after they obtain the volume compression. The pressure is calculated with a magnetohydrodynamic computer code.

The initial volume of the sample was 14.1 cm^3/g, so that the volumetric compression was about 14. Pressure goes as high as 3.5 megabars and then relaxes in about 0.5 microsec to 1.5 megabars.

Theoretical predictions for the transition density, Grivorev and his collaborators say, range between 0.5 and 1 g/cm^3 while the pressure value ranges between 0.25 and 18 megabars. Hawke told us that the best theoretical estimate for a lower limit on the pressure is 1.7 megabars with an error bar of -0.3; an upper limit is very difficult to obtain, he says. This calculation is based on recent shock-wave results from Livermore and Los Alamos. Neil Ashcroft (Cornell) has predicted that the most likely transition pressure is 1.6 megabars.

There are also attempts to achieve metallic hydrogen with static presses. One effort is at Cornell, where Arthur Ruoff is trying to obtain 3 megabars with a static press. He recently did a calculation based on plasticity theory that shows that several megabars can be obtained using steel or sintered tungsten carbide. A proposed program, at the University of Maryland, is headed by Ian Spain. In the Soviet Union Leonid Vereschagin at the Institute of High Pressure Physics has discussed a 10-story-high static press, which is apparently intended to make large sintered diamonds. However he also plans to use the press to reach 2–3 megabars and attempt to make metallic hydrogen. Unlike the dynamic experiments, the static experiments would allow one to recover the metallic hydrogen if it is metastable and if they are capable of reaching the transition pressure. Vereschagin, using a different static press, said he has so far been able to reach 2.5 megabars (compared to the 2.8 megabars reported in the dynamic experiment by Grivorev and his collaborators) with a stiff sample. Hawke notes that the hydrogen is elastically very soft and must be studied at cryogenic temperatures, making it much more difficult to reach the required pressure.

If metallic hydrogen turns out to be metastable, it would of course be very useful to have metastable deuterium in particular. One can envision applications in weapons, controlled fusion and laser fusion. And the possibility some theorists have raised that metallic hydrogen could be a room-temperature superconductor has certainly evoked interest in making the substance. Even astrophysicists are interested in metallic hydrogen because it is possible that it occurs in the interior of Jupiter and Saturn and in white dwarfs.

To use metallic hydrogen on earth may be very tricky indeed. As Hawke told us, the stored energy in metallic hydrogen is very high, 30–40 times greater than that of TNT, so that if metallic hydrogen is metastable it will be extremely dangerous. —GBL

Report reviews studies of mid-Atlantic ridge

A new report, *Understanding the Mid-Atlantic Ridge,* has been issued by the National Academy of Sciences. The report outlines an orderly approach to a comprehensive study of the Mid-Atlantic Ridge. It reviews present knowledge and hypotheses, states major unsolved problems and possible methods of solution, and presents outlines of recommended programs, including general priorities of the programs, coordination of necessary joint projects, and estimates of new funds and facilities required. □