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NEUTRONS HELP US UNDERSTAND THE STRUCTURE OF MATERIALS

Although the existence of the neutron was established by Sir James Chadwick at Cambridge in 1932, it was not until the end of World War II that the increased fluxes of neutrons available from nuclear reactors made it feasible to use them in the study of condensed matter. Fortunately, the foundation for understanding the relation between the diffraction patterns formed by neutrons scattered from crystals, amorphous solids, liquids and large scale structures had been well layed by the earlier discovery of X-rays by Röntgen in 1895, the demonstration of their diffraction by a crystal by von Laue in 1912 and the pioneering efforts in the determination of atomic arrangements in crystalline materials begun in 1913 by Sir Lawrence Bragg.

Both X-ray and neutron radiation can be produced with wavelengths comparable with the distances between atoms in solids, 1-3 Å or 0.0000001 millimetres, and will therefore be diffracted through sizeable angles. The scattering mechanism is however different for the two radiations. X-rays are scattered by all the electrons in an atom whereas neutrons interact both with the nuclei at the centre of atoms and also, because the neutron has a magnetic moment, with the atomic origins of magnetism principally associated with a few of the outer electrons in a restricted number of elements.

X-ray sources are many orders of magnitude stronger than even the best neutron souces such as **ISIS**, but the scattering power of an atom for X-rays or neutrons is roughly comparable. The fact that most materials absorb neutrons much less than X-rays is therefore crucial, since it enables us to use much larger samples than is possible in X-ray work and, consequently, to complete experiments in a reasonable time (a period of hours or days).

Why do we bother to use neutrons if X-rays are generally cheaper to produce and are much more abundant? Several factors make the neutron an invaluable tool with which to complement the structural information obtainable by X-ray scattering:

- The scattering power of elements, and indeed of isotopes of a single element, varies in a rather random fashion as a function of increasing atomic number Z. This contrasts with the monotonic increase in X-ray scattering power, which is proportional to the number of atomic electrons, from Z=1 in hydrogen to 92 in uranium. It is generally easier to study compounds containing both light and heavy atoms with neutrons, since with X-rays the scattering of the heavy elements is dominant.

- The nucleus is effectively a point scatterer, being some hundred thousand times smaller than the wavelength of the neutrons being scattered. This means that the nuclear scattering remains constant as the angle of scattering increases and the resulting diffraction patterns are measurable over the whole range from forward to backward angles. The scattering of X-rays is reduced as the scattering angle is increased because the scattering objects, the atomic clouds of electrons, have much the same dimensions as the wavelength of the incident radiation. The determination of the parameters which describe the thermally-induced vibrations of atoms about their mean positions is much more precise when obtained from neutron data.

. The unique role of hydrogen in stabilizing biological and other molecules through hydrogen bonding, together with its presence in most organic compounds, make its structural location of paramount importance though difficult to determine by X-ray methods. In this respect, neutrons are especially powerful since hydrogen scatters as strongly as many other elements. In addition, the availability of deuterium, the isotope of hydrogen of weight 2, which has a very different scattering power allows us to 'label' specific parts of molecules for subsequent identification. Again, heavy water/light water mixtures can be used to contrast-match specific volumes of large hydrogenous structures in solution: this removes their contribution to small-angle scattering and helps in their structural identification.

If we add to these qualities the special contribution that neutron scattering makes to our knowledge and understanding of magnetic structures and, at a more detailed level, of the spatial distribution of magnetization within solids, then it is easy to see why neutrons are so important in solid state physics, chemistry and biology.

The diffraction instruments already in use at ISIS are:

. **HRPD** - in many respects the world's best powder diffractometer whose high resolution is invaluable for determining complex structures and for the understanding of subtle phase changes.

. **POLARIS** - a powder diffractometer whose performance is complementary to that of HRPD, offering a higher neutron flux at reduced resolution. Its uses include time-resolved studies of chemical reactions, strain measurement and the determination of structures under high pressure.

. **SXD** - a single crystal diffractometer equipped with three large, position sensitive, area detectors for three-dimensional diffraction surveys.

. **LAD** - for the study of the structures of disordered materials such as gases, liquids, glasses and amorphous solids.

. **SANDALS** - for investigations similar to those undertaken on LAD, but with special emphasis on materials containing light atoms.

. **LOQ** - for the measurement of small angle diffraction to investigate large scale structures (10 - 1000 Å) of a wide variety of materials, many of practical importance such as polymers and colloids.

To these must be added the reflectometer **CRISP**: this instrument has already made significant contributions to the study of the structure of surfaces and interfaces in surface chemistry and magnetism.

Finally, it should be remarked that the modern engineer has also found that neutrons, with their high penetrating power, can provide three dimensional information on the strains in a full-sized engineering component from a non-destructive diffraction experiment and, through neutron radiography, can locate the oil in a running engine and measure the temperature of its internal components.

Bruce Forsyth, May 1990.