Neutron diffraction is a
powerful and often unique tool
for studying the structure of
materials used in everyday life

Introduction – Alan Hewat

Alan Hewat
Head of the
Diffraction Group

New materials are everywhere! Imagine all the tiny magnets in the electric motors of a new car, the lighter, longer-lasting batteries that power a mobile phone or computer, the selective catalysts used to create new fuels and clean up the environment. Imagine machines made from new kinds of fibres, with motors made from novel ceramics – both lighter and tougher than the metals they replace. Imagine storing greenhouse gases at the bottom of the ocean, or finding vast reserves of energy in this 'inner space'. But who could imagine, a few years ago, new superconducting materials that could conduct electricity without loss, and be used in more powerful magnetic scanners to map the human body in the finest detail? Who can imagine the future without working on the materials that will make it possible?

The properties of these materials are largely determined by their structure – structure on the atomic scale, or nano-structure (see Box). The distance between atoms is only about 0.1 of a nanometre (nm or one-billionth of a metre) much smaller than the wavelength of light (100 to 200 nm), so clearly we cannot use light. But neutrons, along with electrons and X-rays, can provide a new kind of 'microscope'. Neutrons are subatomic particles that act like waves – like X-rays, and electrons. Since the wavelength of 'thermal' neutrons is similar to the distance between atoms, they have the potential for providing images of structure on an atomic scale.

Neutrons – an ideal probe of materials

Neutrons have many useful properties:

- Neutrons are electrically neutral, unlike electrons, which have a negative charge. They can therefore penetrate deeper inside materials, and are even more penetrating than X-rays. This can be important for 'non-destructive' measurements of engineering components, and materials under extreme conditions such as inside pressure cells, furnaces and refrigerators;

- Neutrons interact with the tiny central nuclei of atoms, while X-rays are scattered by the surrounding clouds of electrons. Neutrons can then locate atoms more precisely, and scattering is strong even at high scattering angles;

- Most important, neutrons act like tiny magnets, and are a unique tool for determining the magnetic structure of materials;

- Finally, the energy of thermal neutrons is similar to the energy of vibration of atoms in solids, and other types of 'excitations' involving magnetism. So neutrons can be used to study the dynamics of materials, and the forces between atoms.

What kind of experiments can we do?

We generally use a large crystal monochromator to select a particular neutron wavelength, just as the different wavelengths of light can be separated using a prism or fine grating. The material to be studied is placed in this monochromatic neutron beam, and the scattered neutrons are collected on a large 2D detector. The sample can be a liquid, a bunch of fibres, a crystal or a polycrystal. A polycrystal is the usual form of solid matter, such as a lump of metal or ceramic, and is made up of millions of tiny crystals.

To understand how neutron diffraction works, imagine how light is diffracted by a regular grating or grid. Scattering from the different lines of the grid interferes to give diffraction 'spots' with spacing inversely proportional to the spacing of the lines. X-ray and neutron diffraction work the same way, but the grid is now the array of atoms in the material. By measuring the intensities and positions of the scattered X-ray or neutron spots, we can deduce the atomic structure.

Neutron diffraction experiments at ILL are thus really quite simple, and available to a wide variety of users – materials scientists, chemists, physicists and biologists. The simplest is called ‘powder diffraction’, when a polycrystalline lump of material, often ground to a fine powder, is placed in the beam. Neutrons are scattered at specific angles, corresponding to the spacing between atomic planes, and by measuring these angles and intensities the atomic structure of the material can be deduced. If instead of a crystalline powder an amorphous or liquid sample is used, there are only broad peaks at specific angles corresponding to average interatomic distances.

To obtain more data, short neutron wavelengths are used, and sometimes one type of atom is replaced by its isotope – chemically identical, but with a different nucleus and different neutron-scattering power – this difference then gives information specific to that atom. So-called inelastic scattering is a little more complicated. Here the change in neutron energy is measured as well, and this gives information about the energies of vibrations and other excitations in the sample.

How can we obtain more neutrons ?

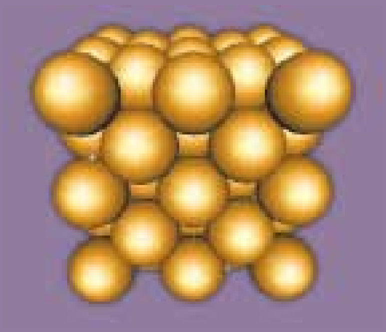
Although neutrons are the ideal probe for studying the structure of materials, the number of neutrons (even at the Institut Laue-Langevin, ILL, in Grenoble – the world’s highest flux neutron source) is still only a tiny fraction of the number of electrons in the beam of an electron microscope, or the number of X-ray photons from X-ray sources.

It would be expensive to build a more intense neutron source, but cost-effective to make better use of the source that we already have. This is not as difficult as it might seem. Today, most neutrons are wasted because our detectors are small. New types of detectors, being developed at ILL and elsewhere, can increase the number of neutrons that we actually count by a factor of 10 or more.

The ILL is also developing new neutron optical elements, such as focusing monochromators and super-mirror neutron guides (which act like optic fibres for light), to bring more of the available neutrons to samples. These techniques are particularly important for the study of structure with neutrons, since new materials are often only available in small quantities when first produced. □

Why structure is important

The influence of structure is everywhere; the properties of water and ice, the hardness of metals, the strength of magnets, and even the biology of DNA or the effect of antibodies on viruses – all depend on structure. For example, the structure of gold consists of close-packed atoms, much like a stack of oranges in the local supermarket. The planes of oranges can easily slip over each other, and for largely similar reasons gold is readily malleable. There is another slightly less close-packed structure in which atoms are arranged at the corners of a cube, with another atom at the centre. The planes of atoms in this structure can slip less easily, and metals that adopt it, such as chromium, are less malleable. This is a trivial example, and there are other structural reasons why some metals are harder – to do with ‘impurities’ and imperfections, which also pin atomic planes and stop them from slipping. The articles in this booklet show many examples of the relation between the structure and properties of new materials.



The structure of gold, revealing its ‘stack of oranges’ arrangement