Fibre Diffraction

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X-ray and neutron fibre diffraction methods provide highly complementary information at relatively high resolution (2-3Å) for a wide variety of biological and industrial polymer systems. While x-ray methods provide data that is essential for definitive structural work, neutrons provide information on the location of hydrogen atoms or solvent molecules that is not usually accessible by x-ray methods. Such detail may be vital for a full understanding of the relationship between structure and function/physical properties.

The scope of X-ray fibre diffraction is constantly being widened by new synchrotron radiation facilities, offering (for example) opportunities for the study of small samples and for the studies of changing systems at high time resolution. Facilities for neutron fibre diffraction studies of polymer systems are also changing rapidly, both at reactor sources such as the Institut Laue Langevin (ILL) and also at spallation sources such as LANSCE at Los Alamos and ISIS at RAL in the UK. Neutron fibre diffraction was originally developed at the ILL on instrument D19 for the study of hydration patterns in polymeric DNA. The method has also been used to carry out work on other fibrous biological systems including cellulose hyaluronic acid and filamentous viruses. All of the studies have relied on the fact that hydrogen and deuterium scatter neutrons more strongly than they do x-rays. Consequently it is possible to locate solvent molecules, bound ligands, or even individual hydrogen atoms within polymer structures in a way that is not possible using x-ray diffraction. The ability to deuterate samples either selectively or non-selectively also adds a dimension to this type of work that is largely inaccessible using other techniques; the formation of a new deuteration laboratory within the ILL/EMBL is therefore highly significant for this type of work.

This lecture will describe the basis of fibre diffraction and give examples of the type of work carried out with x-ray and neutron methods.