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Bragging about Crystallography

Speakers:

Prof Elspeth Garman, Laboratory of Molecular Physics, Dept of Biochemistry, University of Oxford.
Professor Emeritus Sir Thomas Blundell, previously Head of Dept of biochemistry, University of Cambridge.

The talks covered a little history of X-ray cystallography plus the contemporary work on drug design but did not give an overall account. I have tried to fill in.

To begin: in a poll organised by a cluster of British Science, Technology and museum organisations 50,000 people voted X-Ray Crystallography as the third top past British innovation. [top was Alan Turin's universal machine]

To my mind X-Ray Crystallography is rather an international affair, as will unfold. The history of Crystallography is a wonderful story of a succession of scientists hugely changing many arenas of science.

Humans have been interested in stuff that comes out of the ground for thousands of years - stone for building, coal for providing heat, iron, copper, tin, zinc to produce metal alloys for tools, weapons, armour, gold, silver and gemstones for decorations. Gradually the science of mineralogy developed and by the 17th century the modern study of mineralogy using crystallography and microscopic study of rock sections had developed.

As we know there are 118 elements but only 80 natually occuring stable elements. Elements can combine to form compounds which occur in the ground as solid crystalline substances. 4900 minerals have been identified. Examples, rock salt, anthracite, bauxite, barium, mica, calcite, chalk, metal compounds, graphite, diamond, sulphur, quartz, talc, gypsum, ...
Until the late nineteenth century in crystallography great attention was paid to physical features such as optical properties, cleavage, colour etc , and especially the defining property of a crystal - its symmetry. Seven distinct 'lattice' systems exist based on crystal shapes e.g. cubic, hexagonal and so on.

The big step forward came with the accidential discovery of penetrating rays by Wilmhelm Roentgen in 1885. He did not know what they were and called them X-rays.

There followed a series of remarkable scientists working in the field to understand effects of X-rays on materials.

Max von Laue 1879 - 1960 was a German physicist who wrote his Ph.D thesis on interference phenonema in plane-parallel plates through which rays of light were directed. Laue realised that X-rays must have wave-lengths millions of times smaller that light. He was told about crystals by a young student - he did not know about them and intuited that X-rays travelling through crystals would be diffracted as light is through plane-parallel plates. Experimentalists proved him right and he won a Nobel prize in 1914 for his discovery.

Incidentally, he studied under Max Planck - who gave birth to quantum theory and also worked with Einstein.

William Henry Bragg was born in UK and in 1885 at 23 was appointed Prof of Mathematics and Physics at University of Adelaide where his son William Laurence Bragg was born. The Bragg family returned to UK in 1908 and William Henry, the father, became Cavendish Chair of Physics from 19090. His son, Laurence, an able student, entered Trinity College, Cambridge in 1909 and later transfered to physics and graduated with First Class Honours in 1911.

Father and son continued working together on X-ray crystallography, though in different universities, and from 1912 to 1914 carried out a series of ingenious experiments in X-ray crystallography.

Laurence is most famous for his law on X-ray diffrraction which makes it possible to calculate the positions of atoms in a crystal [1912].

The team shared a nobel prize in 1915: the only father and son team to have done so. Laurence is still the youngest person to have received a Nobel Prize. He was 25.

Laurence was Director of the Cavendish Lab when Crick and Watson were using X-ray diffraction on DNA. which resulted in their Nobel Prize.

John Desmond Bernal 1901 - 1971 is considered a pioneer in X-ray crystallography in molecular biology. At Cambridge, he wrote a lengthy mathematical paper on crystal structure.

He began research at the Faraday Lab under Sir W.H. Bragg after graduation in 1922. He was appointed first lecturer in Structural Crystallography at Cambridge, becoming Assistant Director at the Cavendish Lab. in 1934. He led research on cholesterol, vitamin B1, pepsin, vitamin D2.

Max Perutz 1914 -2002 was Austrian-born British molecular biologist who shared Nobel Prize with John Kendrew for their studies on haemoglobin on which Perutz spent most of his career. He wrote " crystallography shows why blood is red, grass is green, diamond is hard, wax is soft and silk is strong." He worked at the Cavendish Lab, Cambridge under J.D.Bernal.

X Ray crystallography had by this time become the principle method for determining the atomic and molecular structure of a crystal. A fine X -ray beam was directed at a small crystal which diffracted it in many specific directions. The directons of diffraction are measured accurately. Braggs law is then used to compute atomic structure.

In recent years beams of neutrons or electrons have sometimes been used in place of X-rays.

Thus Crystallography has become the science of condensed matter with emphasis on the atomic or molecular structure and its relation to physical and chemical properties.

At first chemists were upset by the results because atoms seem to appear in lines and no molecules could be identified. But eventually the chemists accepted the validity of X-ray crystallography results.

Another interesting aspect of the field has been the preponderance of successful women X-ray crystallographers. and that is still the case.

Dorothy Hodgkin 1910 - 1994 was a British chemist working under J.D.Bernal, where she became aware of the technique's application to determine structures of proteins. She confirmed the structure of penecillin, and was awarded a nobel prize for the structure of B12, using this technology.

You notice the use of X-ray crystallography has now been widened to include organic materials. In fact Perutz [mentioned earlier] worked for 25 years under the sponsorship of the Braggs on Haemoglobin to win his nobel prize.

And of course, as mentioned earlier, Watson and Crick were working under Laurence Bragg when they won their Nobel prize for their work on DNA.

Crystallography continues to move on. Atomic structures, even with thousands of atoms, can now be understood almost immediately using intense light sources [such as the UK's national synchrotron Diamond light source in Oxfordshire].

The range of materials being analysed is now very wide: chemicals, some esoteric organo-metallics, engineering materials, proteins, enzymes, pharmaceuticals, and may other organic and biological chemicals. It is used in engineering, metallurgy, pharmaceutical design and analysis.

It uses extensive maths and computing.

Thus it is an incredibly fruitful technique used across the whole engineering and science spectrum.

And the Cavendish is still at the cutting edge.