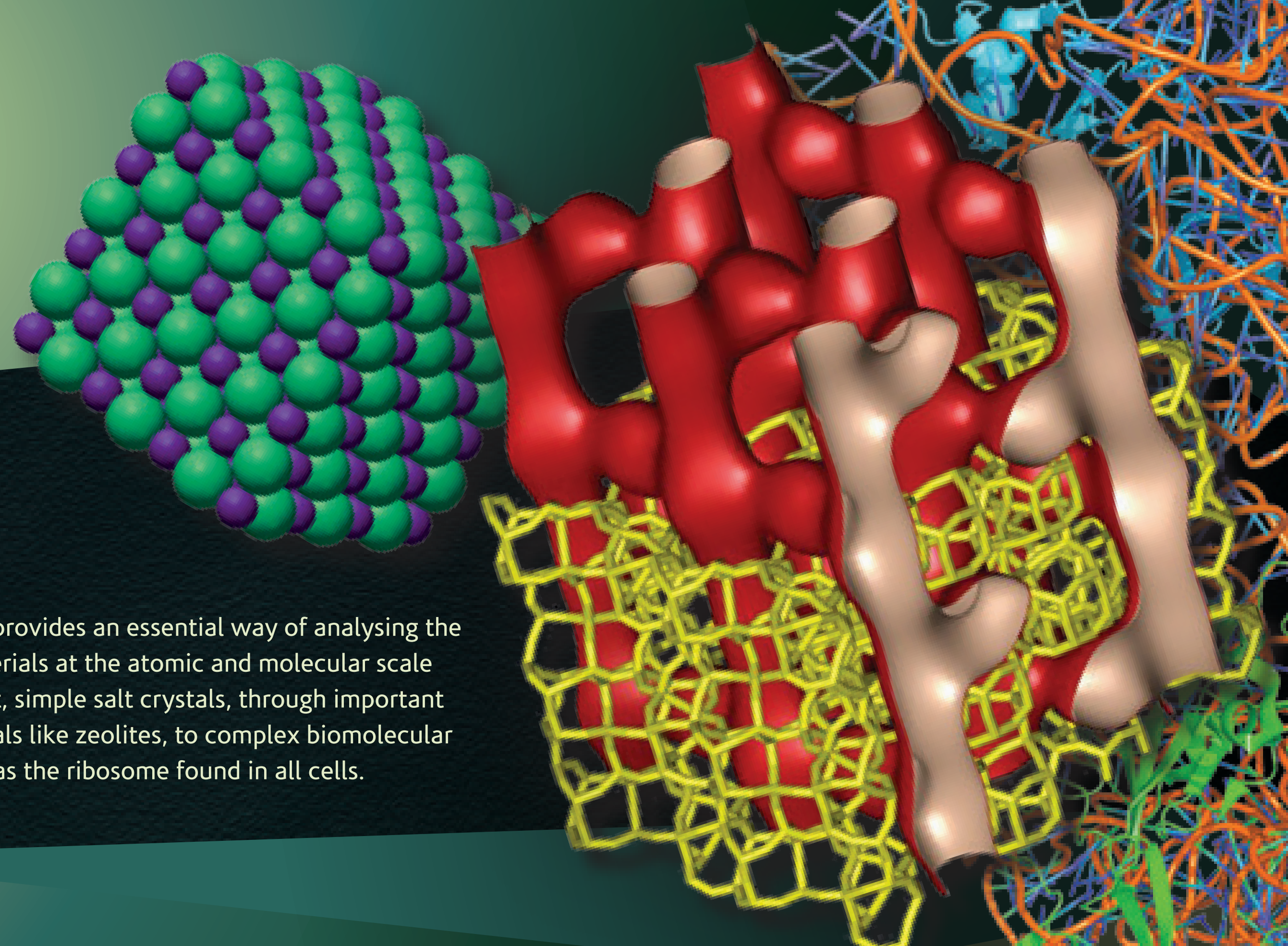
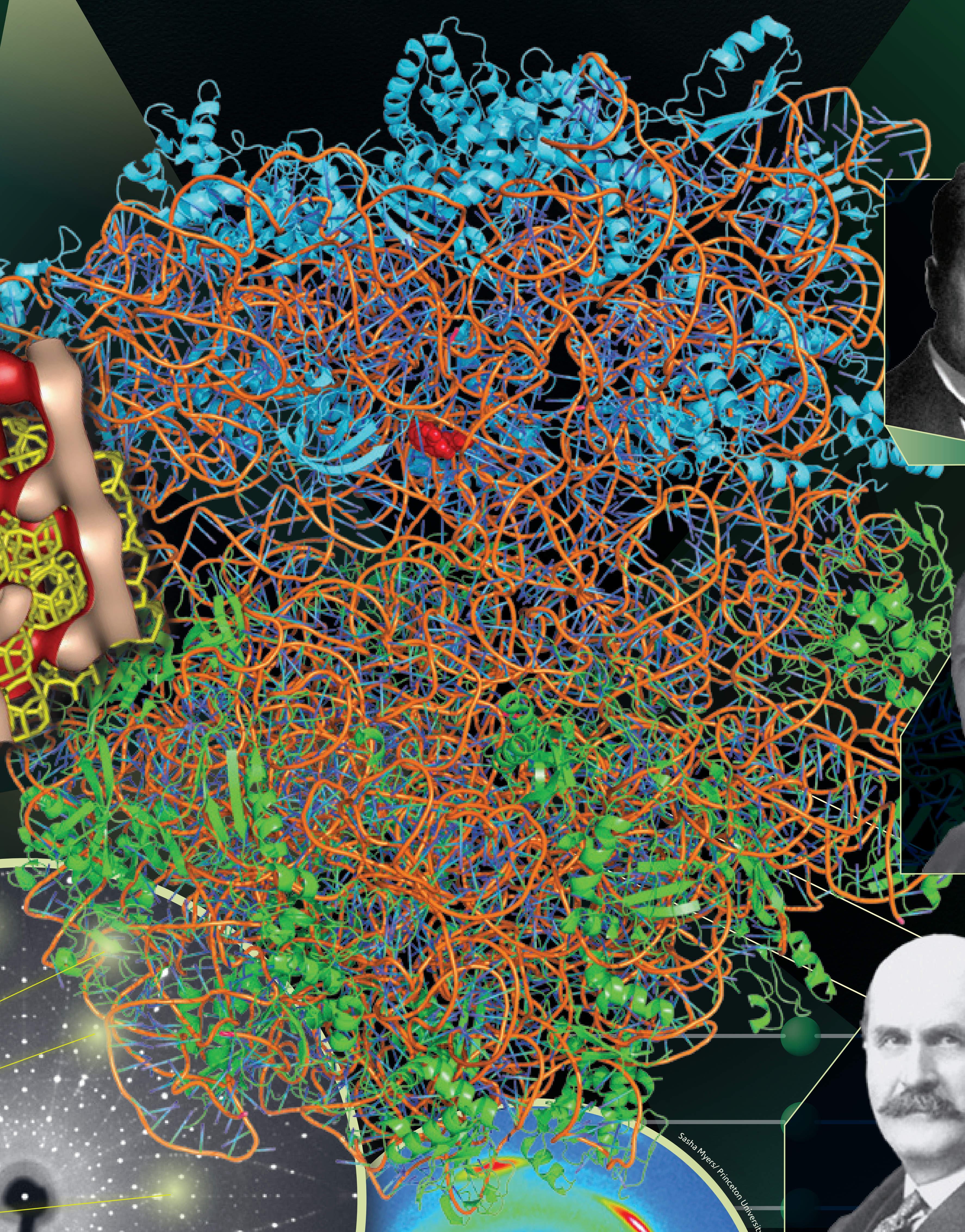
Atoms illuminated

One hundred years ago, two scientists in the UK pioneered a method for uncovering how the atoms in a crystal were arranged. The science of **crystallography** was born.



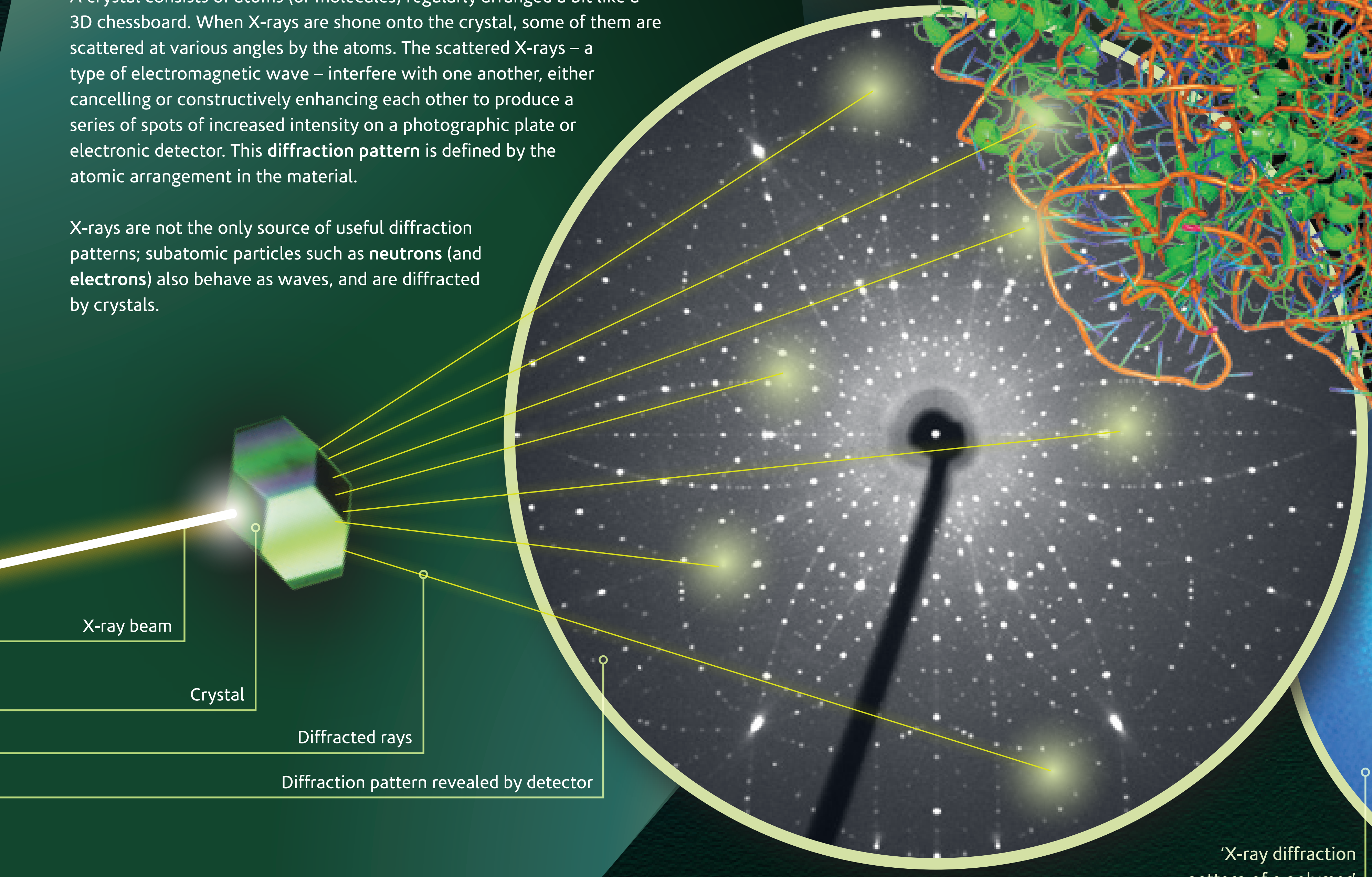


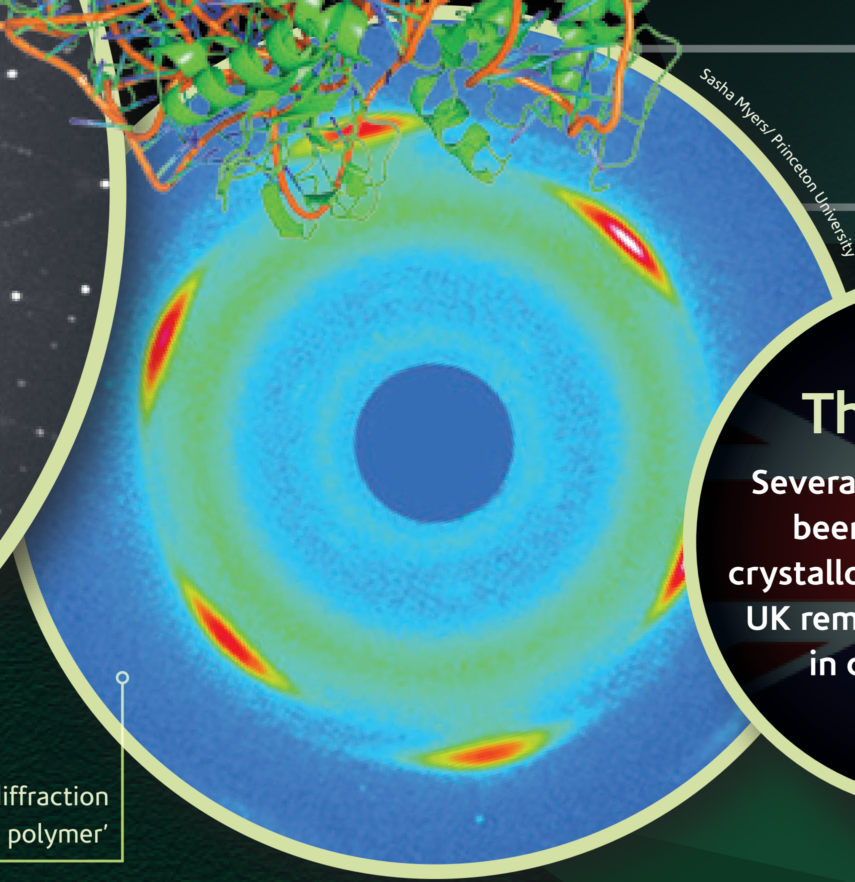
Crystallography provides an essential way of analysing the structure of materials at the atomic and molecular scale from, left to right, simple salt crystals, through important industrial materials like zeolites, to complex biomolecular assemblies such as the ribosome found in all cells.

What is crystallography

A crystal consists of atoms (or molecules) regularly arranged a bit like a 3D chessboard. When X-rays are shone onto the crystal, some of them are scattered at various angles by the atoms. The scattered X-rays – a type of electromagnetic wave – interfere with one another, either cancelling or constructively enhancing each other to produce a series of spots of increased intensity on a photographic plate or electronic detector. This **diffraction pattern** is defined by the atomic arrangement in the material.

X-rays are not the only source of useful diffraction patterns; subatomic particles such as **neutrons** (and **electrons**) also behave as waves, and are diffracted by crystals.





Sasha Myers/ Princeton University

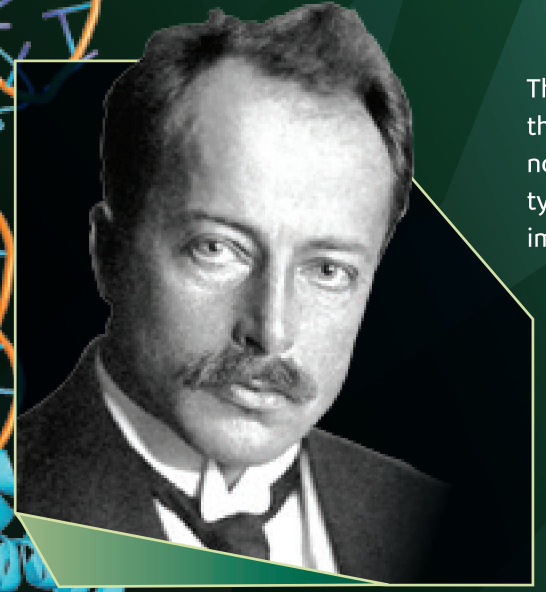
'X-ray diffraction pattern of a polymer'

The UK role

Several Nobel Prizes have been awarded to UK crystallographers. Today, the UK remains a world-leader in crystallography.

Mysterious rays make the perfect tool

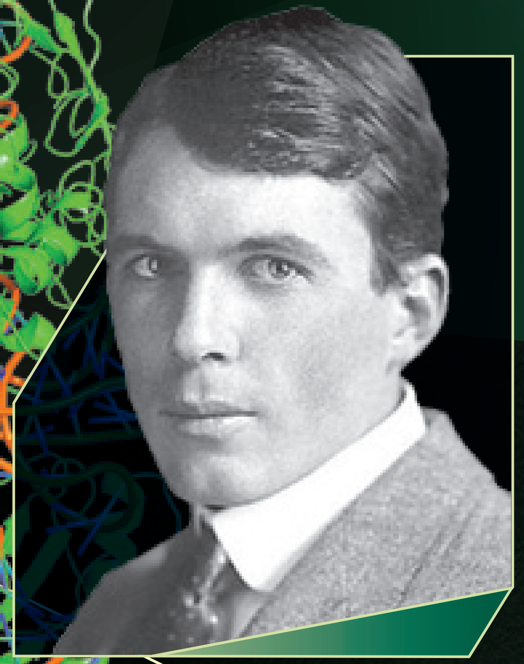
The development of crystallography goes hand in hand with the discovery of **X-rays** by **Wilhelm Röntgen**, who in 1895 noted that a high-voltage vacuum tube emitted an unknown type of radiation, which passed through objects to leave an image on a photographic plate.



Max Laue

The brilliant idea

In 1912, **Max Laue** established that these penetrating X-rays were like visible light, but with wavelengths thousands of times shorter (about 10^{-8}cm). He surmised that these wavelengths would match the regular spacings between atoms in a simple salt crystal such as copper sulphate. X-rays passing through the crystalline array would thus be diffracted.



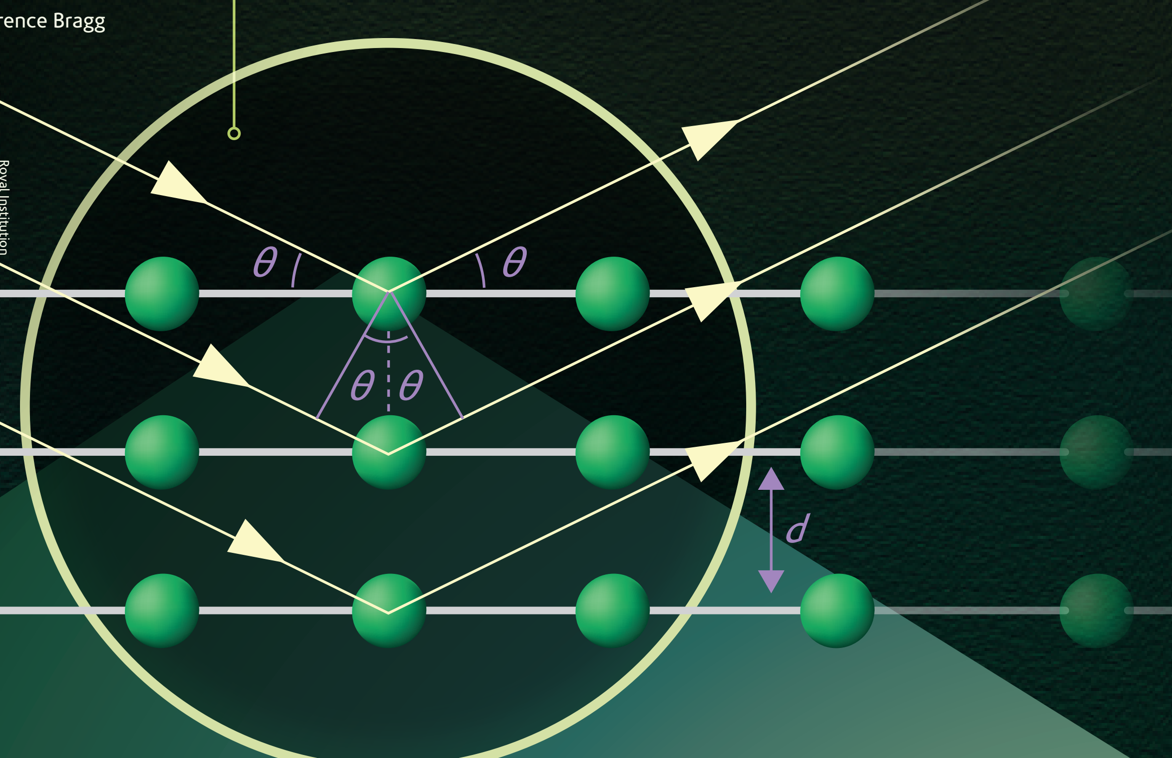
William Lawrence Bragg

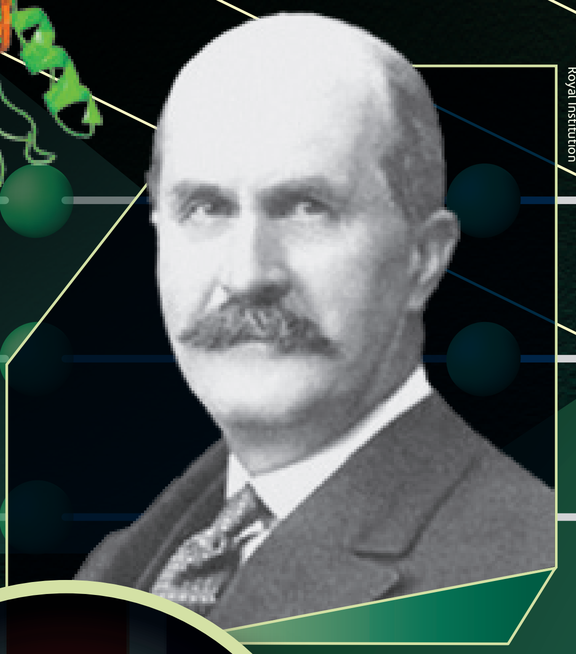
The big solution

How exactly does the diffraction pattern obtained relate to the crystal structure? That was explained by the 22-year old **William Lawrence Bragg** while at the University of Cambridge using a beautifully simple equation known as **Bragg's Law** – which is now the basis of all modern crystallography.

Bragg's Law

Think of a crystal as a stack of sheets of atoms. X-rays reflected from successive sheets then interfere constructively and generate the diffraction spots according to the equation $n\lambda = 2d\sin\theta$ where n is any whole number, λ is the X-ray wavelength, d the distance between sheets, and θ the angle between the incident X-rays and the sheets.





Royal Institution

William Henry Bragg

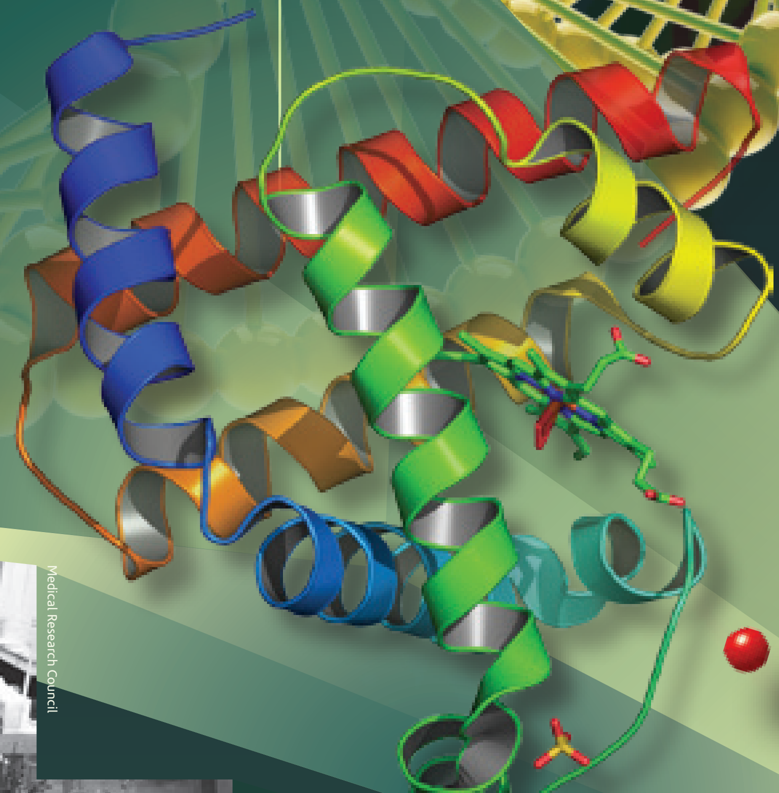
A winning team

Lawrence collaborated with his father, **William Henry Bragg**, who invented a spectrometer that could provide X-rays at particular wavelengths, and allow the intensities of the spots produced to be measured while a sample crystal was rotated around any angle. Father and son solved the structures of several crystals including common salt and diamond. They were awarded the Nobel Prize for Physics in 1915.

A century of crystallography

Molecular biology is born

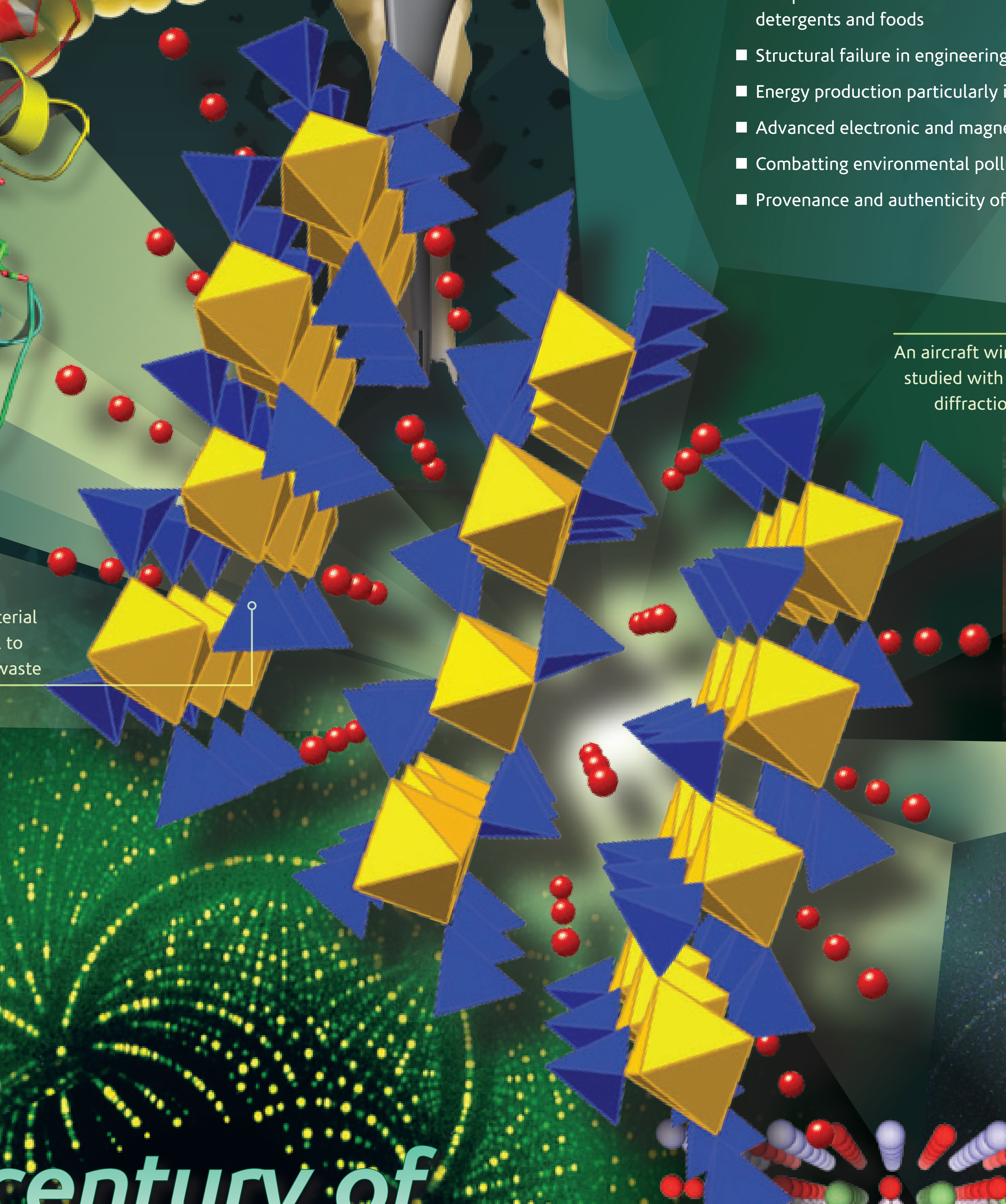
X-ray diffraction has transformed our knowledge of biology through analysing the complex structures of **proteins**, **DNA** and other biomolecules. The crystals have to be painstakingly grown – and while the first protein crystal structures took literally decades to work out, thousands of protein structures are now routinely determined every year.



'Myoglobin, a protein found in muscle tissue

Max Perutz and **John Kendrew** in Cambridge were awarded the Nobel Prize for Chemistry in 1962 for solving the first X-ray structures of key proteins, **haemoglobin** and **myoglobin.**

With brilliant insight, **Francis Crick** and **James Watson**, also in Cambridge, uncovered the DNA double helix from its X-ray pattern, a discovery that led to the development of modern genetics.



Structure of a material with the potential to clean up nuclear waste

What has crystallography done for us?

Crystallography underpins research into:

- Diseases and the development of new medicines
- Catalysts for cleaner, greener chemical manufacturing
- Composite materials such as alloys, ceramics, fibres, plastics, detergents and foods
- Structural failure in engineering and building materials
- Energy production particularly in batteries, fuel cells and solar cells
- Advanced electronic and magnetic materials for new devices
- Combatting environmental pollution and climate change
- Provenance and authenticity of art and archaeological objects

Diamond Light Source

Crystallography today

Crystallography has advanced dramatically in recent decades. Large molecular assemblies or networks, or randomly structured materials can now be studied – in the form of powders, thin films, flowing liquids and large objects, and under varying conditions such as pressure, temperature and magnetic field. The subtle motions of individual atoms and molecules can also be followed.

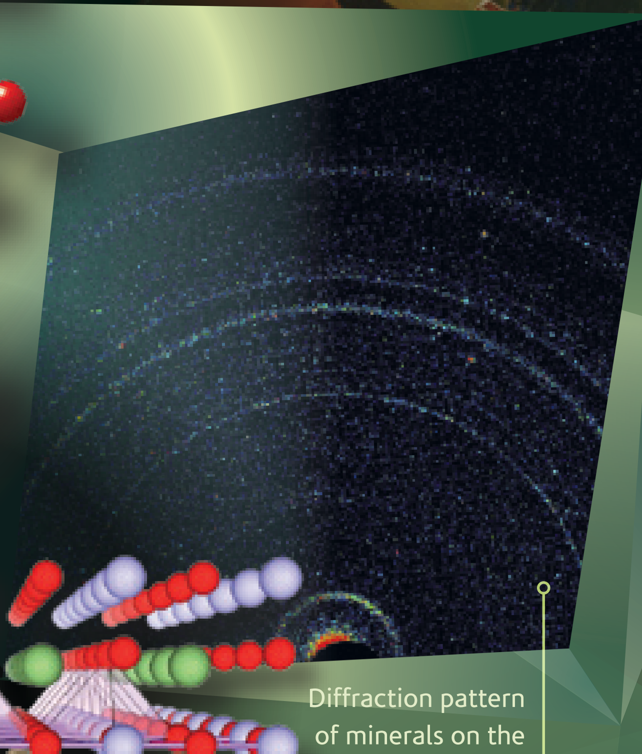
An aircraft wing being studied with neutron diffraction at ISIS

The rise of the machines

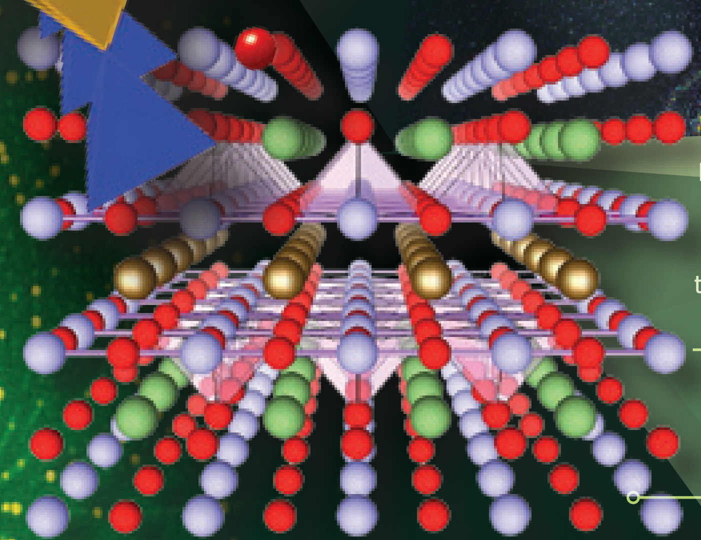
Advanced studies of molecular structures have largely been made possible by the development of powerful, large-scale X-ray and neutron sources that enable many experiments to be carried out simultaneously. Intense X-ray beams are generated using a circular particle accelerator called a **synchrotron** – the **Synchrotron Radiation Source (SRS)** at the STFC Daresbury Laboratory in Cheshire was the first such dedicated facility. The beams' brilliance and pencil-like focus means that much smaller crystals can be studied, which is particularly important in protein analysis where the crystals grown may be tiny. Today, even brighter beams are available at the **European Synchrotron Radiation Facility (ESRF)** in Grenoble, France and the **Diamond Light Source** at Harwell, Oxfordshire.

Neutron beams produced at facilities such as **ISIS** at the STFC Rutherford Appleton Laboratory and the **Institute Laue-Langevin (ILL)** in Grenoble are similarly used to obtain complementary and often unique structural detail.

State-of-the-art digital X-ray or neutron detectors are used to record the diffraction data – and, when combined with advanced computer processing, allow researchers to determine in minutes structures that would have taken months just 20 years ago.



Diffraction pattern of minerals on the Mars surface from the Curiosity Rover diffractometer



Structure of a high-temperature superconductor

Inside modern materials

From the beginning, diffraction has been used to analyse naturally crystalline materials such as metals, alloys, minerals and complex compounds. Diffraction studies can pinpoint impurities and defects in a crystal structure, or probe the subtle magnetic and electronic behaviour that may be key to improving the performance of a functional material.

Women and crystallography

The Braggs actively encouraged women into crystallography, who have excelled in solving many crucially important molecular structures. They are still strongly represented in the field today.

As part of William Bragg's team, **Kathleen Lonsdale** established the structure of a benzene derivative, which confirmed that benzene – a basic unit of many organic materials – was a flat ring.

Dorothy Hodgkin was one of the pioneers of X-ray crystallography applied to biomolecules. She solved the structure of penicillin, vitamin B12 and insulin, winning the Nobel Prize for Chemistry in 1964.

The X-ray diffraction images of DNA meticulously collected by **Rosalind Franklin** led to the determination of its structure in 1953.

Further information

FOR GENERAL INFORMATION:

British Crystallographic Association: http://crystallography.org.uk

International Union of Crystallography: www.iucr.org

http://en.wikipedia.org/wiki/Crystallography

EDUCATIONAL RESOURCES:

www.pcg-scmp.org/Education

www-outreach.phy.cam.ac.uk/camphy/xraydiffraction/xraydiffraction_index.htm

http://escher.epfl.ch/eCrystallography

www-structmed.cimr.cam.ac.uk/course.html

SCIENCE AND TECHNOLOGY FACILITIES COUNCIL:

www.stfc.ac.uk

Diamond Light Source: www.diamond.ac.uk

ESRF: www.esrf.eu

ISIS: www.isis.stfc.ac.uk

ILL: www.ill.eu

Celebrating Crystallography
Bragg Centenary 1913 – 2013

Science & Technology Facilities Council

The UK's Science and Technology Facilities Council operates world-class, large-scale research facilities; supports scientists and engineers world-wide; funds researchers in universities and provides strategic scientific advice to government.

The Council's Public Engagement Programme offers a wide range of support for teachers, scientists and communicators to facilitate greater engagement with STFC science which includes astronomy, space science, particle physics, nuclear physics and materials science. Visit us at www.stfc.ac.uk – Public and schools.

Accompanying teachers' notes are available at www.stfc.ac.uk/teachers

Produced by STFC on behalf of UK organisations.

www.stfc.ac.uk

Science & Technology Facilities Council