



ARC Centre of Excellence for
COHERENT X-RAY SCIENCE



THE UNIVERSITY OF
MELBOURNE

From Moseley's Law to the Molecular Microscope

A century of X-ray physics in chemistry and
biology (1913-2013)

Harry Quiney

19 July 2013

Overview

1. Moseley, Rutherford, Darwin, Bohr and “*the high frequency spectra of the elements*” (1913)
2. Atomic structure and inner-shell X-ray spectroscopy: *the early years.*
3. X-ray scattering and the structure of materials and biomolecules: *the Third Revolution*



CXS: The ARC Centre of Excellence for Coherent X-ray Science

ICHEP, 4 July 2012

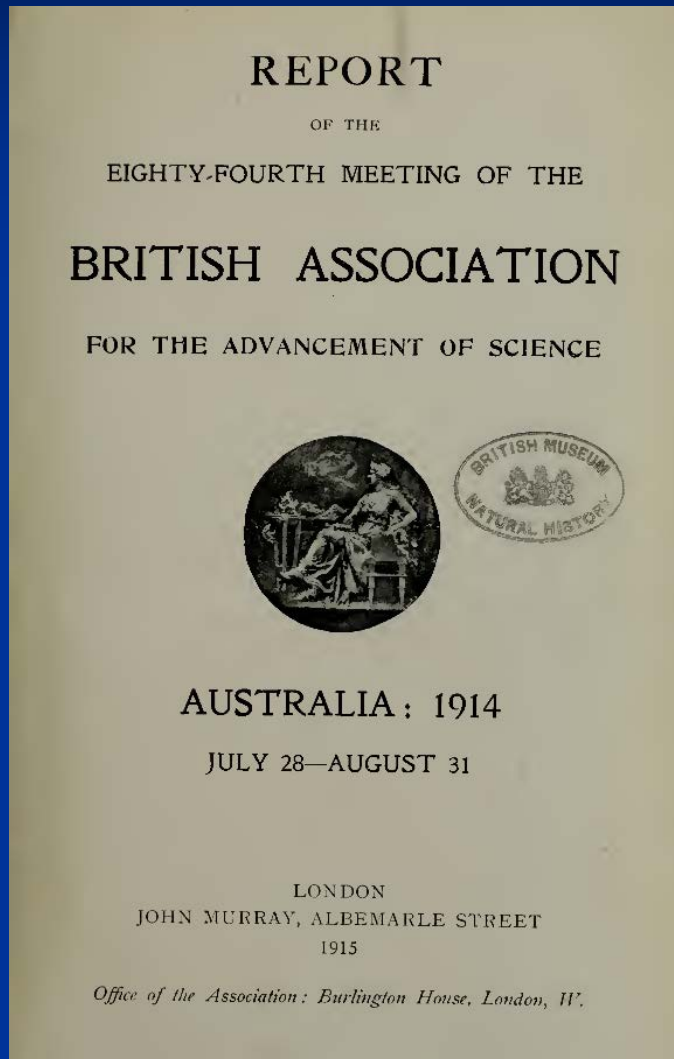


On 4 July 2012, Melbourne was at the host to the world's leading conference in particle physics, ICHEP 2012 (Rochester Meeting)

Using 21st Century technologies, the discovery of the Higgs' Boson was announced live from CERN at the conference, finally confirming the Standard Model.

...certainly not the first time the School of Physics at Melbourne has been the centre of the action!

British Association in Australia (1914)



- Australian Government invested £15000 to host this meeting in Australia (Adelaide, Melbourne, Sydney and New Zealand).
- The 1000 page record is a snapshot of Australian science in 1914
- The delegation was led by Sir Ernest Rutherford and the cutting edge physics of the day was atomic structure, the Rutherford atom, Bohr theory and Moseley's X-ray survey of the elements.

At the School of Natural Philosophy, University of Melbourne, Tuesday, 18 August 1914

Sir ERNEST RUTHERFORD AUGUST 18.

Joint Meeting with Section B (Chemistry)

We have now two powerful methods that aid us in determining the inner structure of the atom—the scattering of high-speed particles in transit through matter, and the vibrations of the interior parts of the atom.

the chemical atom. The atomic theory is no longer merely an hypothesis introduced to explain the laws of chemical combination; we are able to detect and count the individual atoms. We can determine the actual mass of an atom in various ways, and know its value with considerable accuracy. The idea that the atom is an electrical structure received a great impetus by the detection of the electron by J. J. Thomson; and, moreover, the Zeeman effect showed that all atoms must contain electrons. The atomic character of negative electricity is well established; we always find the negative electron, however produced, carrying a definite charge. We have, unfortunately, not the same certainty with regard to the behaviour of positive electricity, for it can only be obtained except associated with a mass comparable with that of a hydrogen atom. In J. J. Thomson's model of the atom the positive electricity was supposed to be distributed throughout a large sphere with the negative corpuscles moving inside it. This hypothesis has played a useful part in indicating possible lines of advance; but it does not fit in with more recent discoveries, which point to a concentrated positive nucleus.

We have now two powerful methods that aid us in determining the inner structure of the atom—the scattering of high-speed particles in transit through matter, and the vibrations of the interior parts of the atom. In C. T. R. Wilson's photographs of the tracks of the α particles through a gas we notice many sudden bends in the paths. In order to account for these deflections I

In modern language:

- SCATTERING: the “structure of matter” including Bragg X-ray scattering from periodic solids.
- SPECTROSCOPY: the “electronic structure” of atoms (Mr H.G.J. Moseley, MA)

This is as true today as it was in 1914 and is the theme of this talk.

At the School of Natural Philosophy, University of Melbourne, 18 August 1914

Professor Armstrong (Chemistry, City and Guilds,
London):

“...the arguments used are so novel and daring, the contentions so original, that at present they (chemists) are not in a position to appreciate, still less to criticize them effectively...

Physicists, unfortunately, in the past have held aloof from chemists; the movement now in progress is, therefore, to be welcomed. Hence the value of the present discussions”.

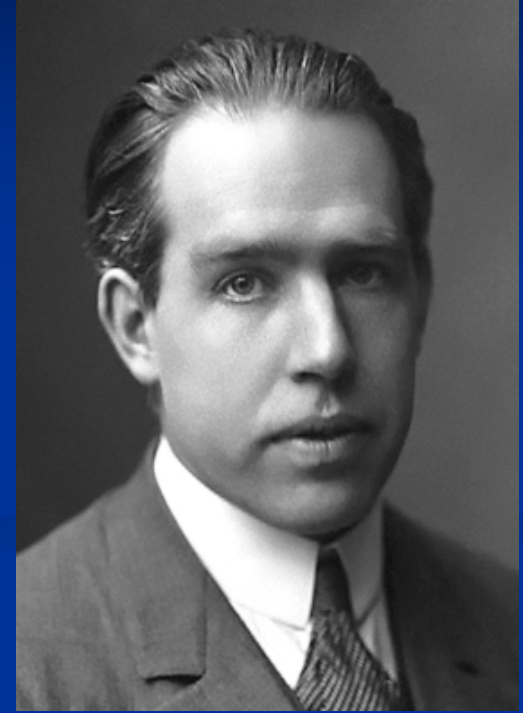
Part I: Moseley, Rutherford and Bohr



Ernest Rutherford 1871-1937



Henry Moseley 1887-1915



Niels Bohr 1885-1962

Bohr-Rutherford Theory (1913)

From earlier July Lectures

- Planck relation: $E=h\nu$
- Rutherford atom: positive charge, Ze , concentrated in a tiny volume (femtometre scale)
- Bohr electron orbits (ångström scale): stationary states constrained by quantized angular momentum, $n\hbar=nh/2\pi$.
- Discrete jumps between levels produce discrete spectra depending on the Rydberg constant, R .

$$h\nu = hcRZ^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Bohr determined R from a theoretical model of hydrogen: the quantum atom

$$R = \frac{m_e e^4}{8\epsilon_0^2 h^3 c}$$

Henry Gwyn Jeffreys Moseley (1887-1915)



H. G. J. Moseley MA, Balliol-Trinity Laboratory, Oxford 1913
(photo: Oxford Museum of the History of Science)

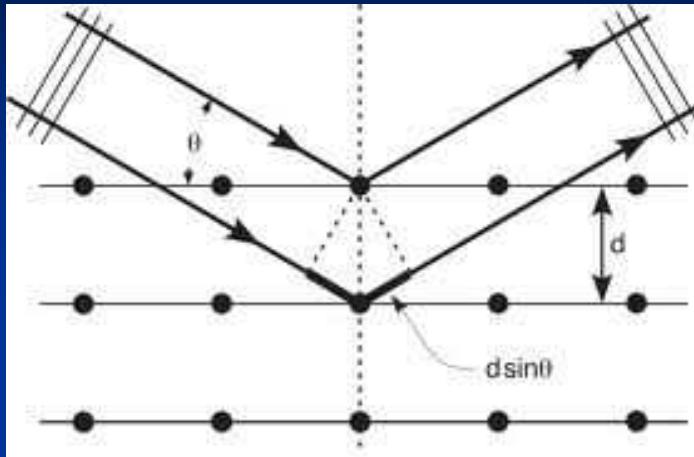
Moseley and Darwin (1912)



- Moseley and Darwin worked together in Manchester under Rutherford to understand the nature of X-rays
- Moseley learned how to generate X-rays by visiting W.H. Bragg in Leeds
- Moseley and Darwin: *Reflection of X-rays by Crystals*, Phil. Mag., **26**, 310 (1913), published with Bohr's atom.

Photo: Charles Galton Darwin (1887-1962), US Library of Congress (1925)

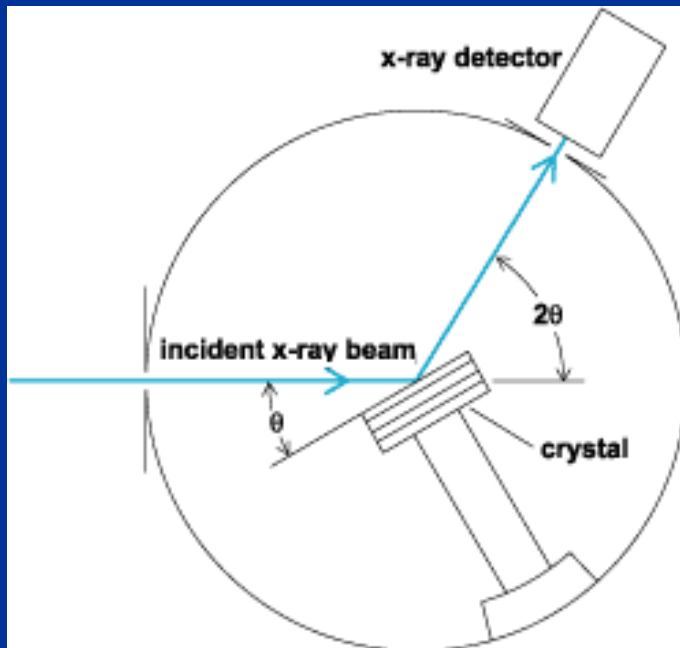
Reflection of X-rays by a Crystal



Bragg's Law: observe constructive interference when

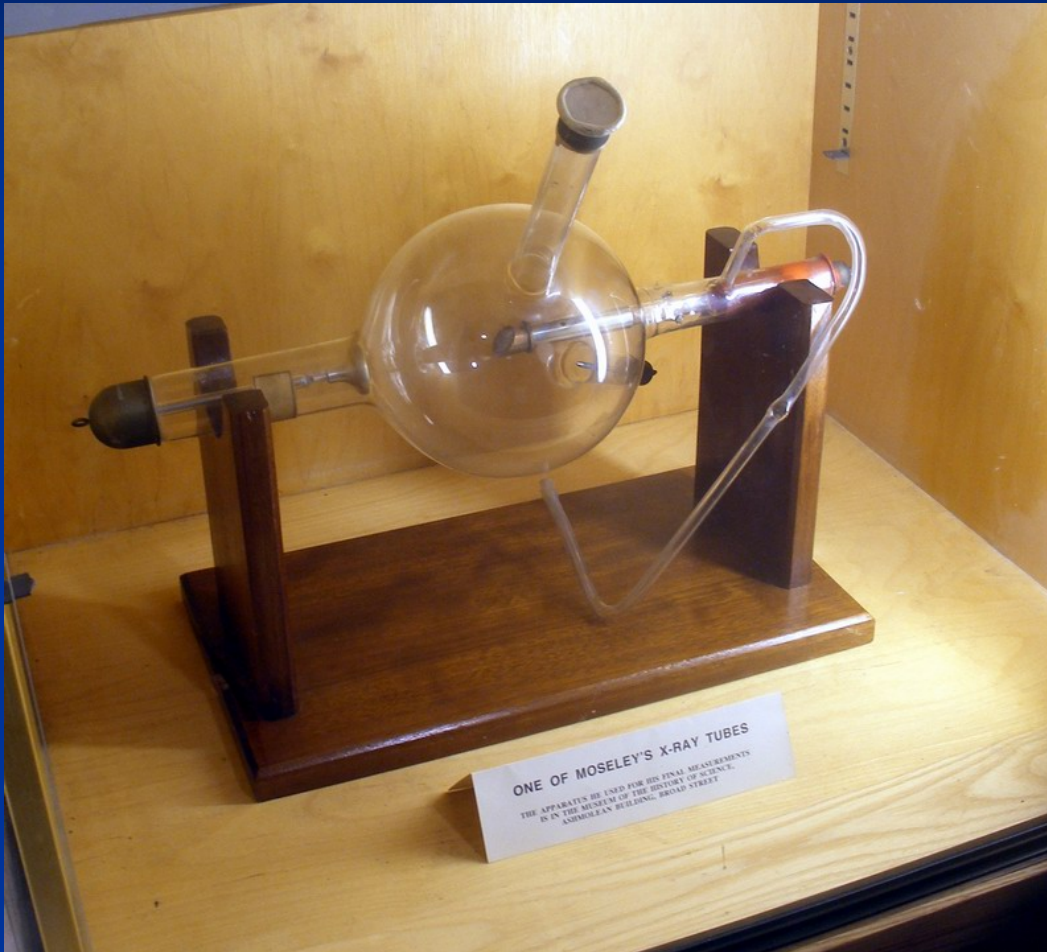
$$n\lambda = 2d \sin \theta$$

Bragg diffraction: with λ fixed, scan through the angle θ with a detector at angle 2θ as shown at left to determine d , the spacing between atomic planes in a crystal.



If you know d , then you can determine λ , and you can use a crystal to build an X-ray spectrometer

Moseley's X-ray Tube

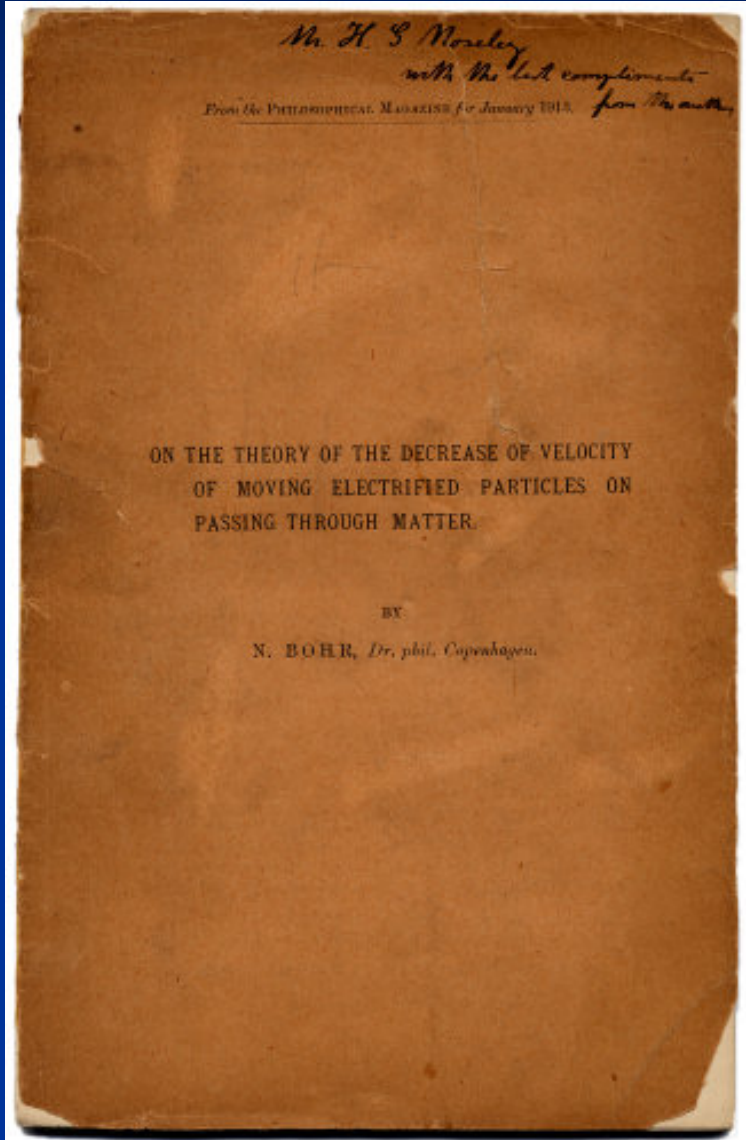


Moseley produced X-rays by bombarding metal targets in a vacuum with high energy electrons

He was able to build his own equipment (a source and a spectrometer) and to swap between different samples very quickly

Image: Museum of the History of Science, Oxford

Moseley and Bohr



- Moseley wrote to Bohr from Oxford on 16 November 1913 describing his preliminary results on determining “the high-frequency spectra” of the elements.
- Moseley described the results as “extremely simple and largely what you (Bohr) would expect”.
- Even though there was not yet a manuscript, Moseley told Bohr that the results would appear in Phil. Mag., December 1913.
- Rutherford saw to it.

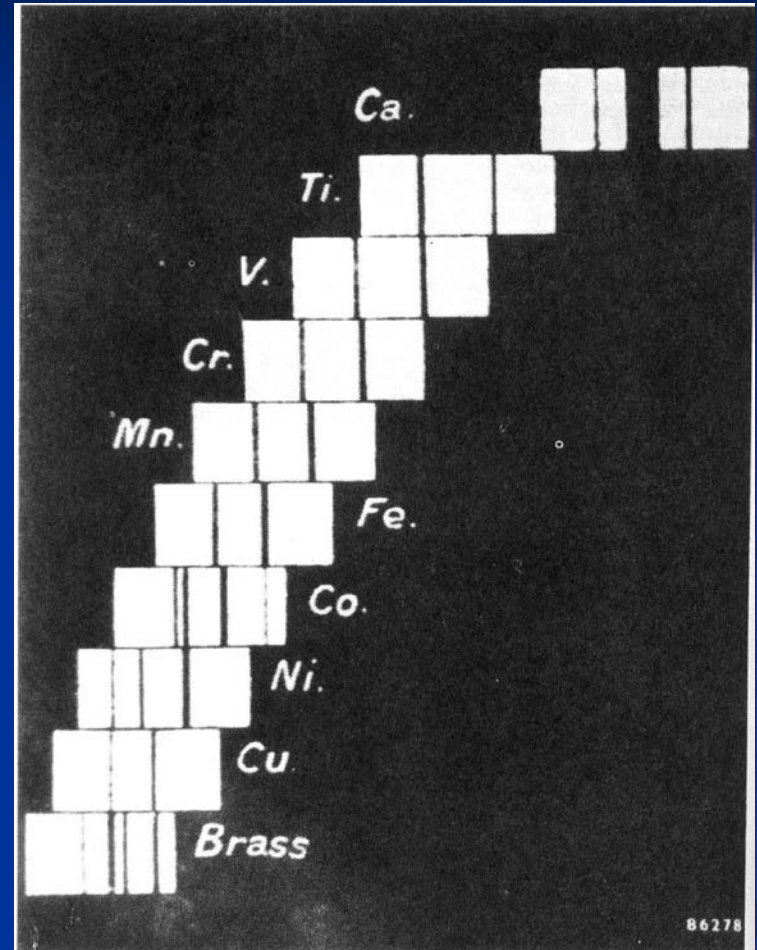
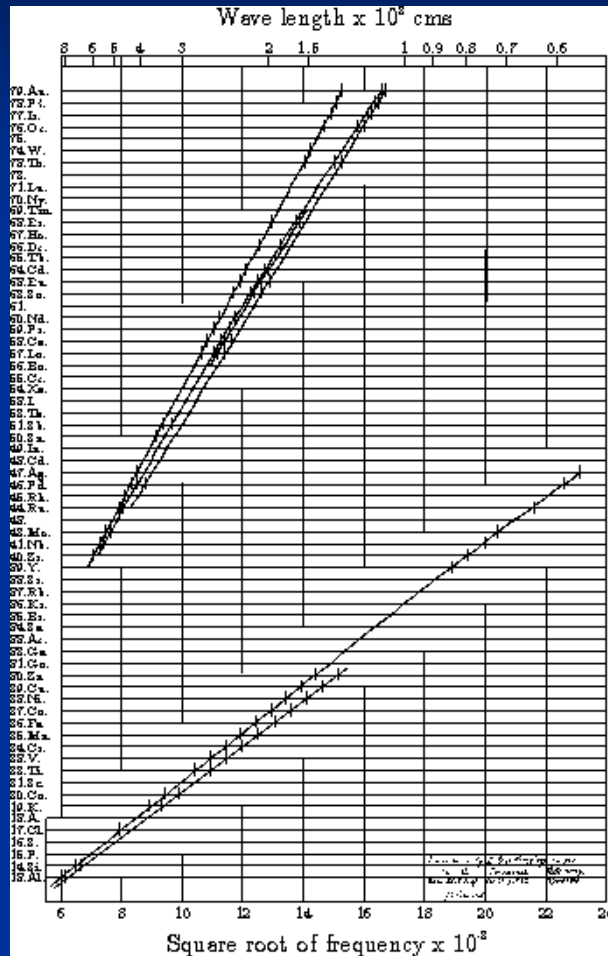
Moseley's Law

$$\nu_X = \frac{3}{4} cR(Z - 1)^2$$

- ν_X is the frequency of the emitted X-ray
- R is the Rydberg constant
- Z is the atomic number (an *integer*)
- c is the speed of light

H. G. J. Moseley, High Frequency spectra of the elements I, Phil Mag, 26, 1024 (1913).

Moseley's Survey of the Elements



H. G. J. Moseley, High Frequency spectra of the elements II, Phil Mag, **27**, 703 (1914).

Moseley's Survey of the Elements

- Broek's hypothesis: Atomic number, Z , is the nuclear charge (Ze), an integer multiple of the electron charge.
- Periodic Table of Elements is organized by Z , not atomic weight, A
- X-ray lines provide direct evidence for Bohr theory.
- Resolved the positions of cobalt (27) and nickel (28)
- Predicted the existence of technetium (43), promethium (61), hafnium (72), rhenium (75).
- Only 15 elements lanthanum to lutetium (lanthanides).
- Identified some "elements" as isotopes (eg radium-B was really lead-207); established the reality of isotopes.
- Exhibited relativistic effects (K_α & K_β fine-structure)

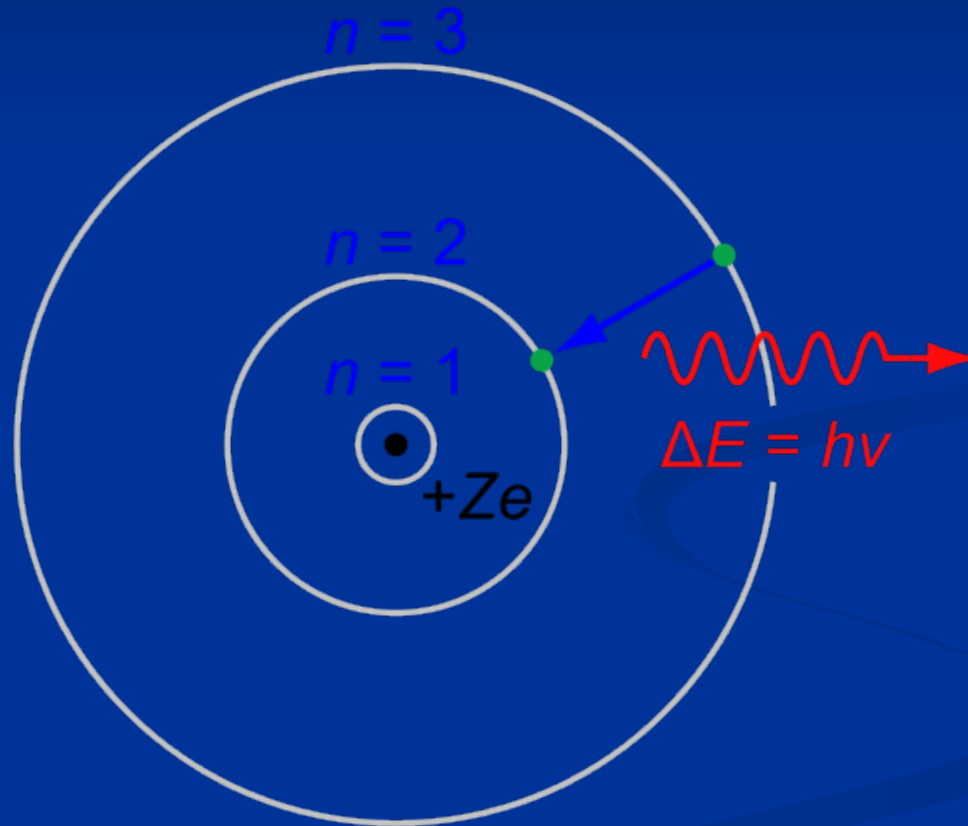
X-ray Nobel Prizes

- 1914: Max von Laue: X-ray diffraction
- 1915: W.H. Bragg and W.L. Bragg: X-ray diffraction from crystals
- 1916: *no prize awarded*
- 1917: Charles Barkla: X-ray spectroscopy

Rutherford and Bohr both credited Moseley with having made atomic structure “respectable”.

There remains widespread speculation that he would have won the Nobel Prize (Chemistry or Physics), had he not been killed, Gallipoli, 15 August 1915.

Part II: Atomic Structure and Inner-Shell Spectroscopy



Walther Kossel (1888-1956)



Walther Kossel (1928)

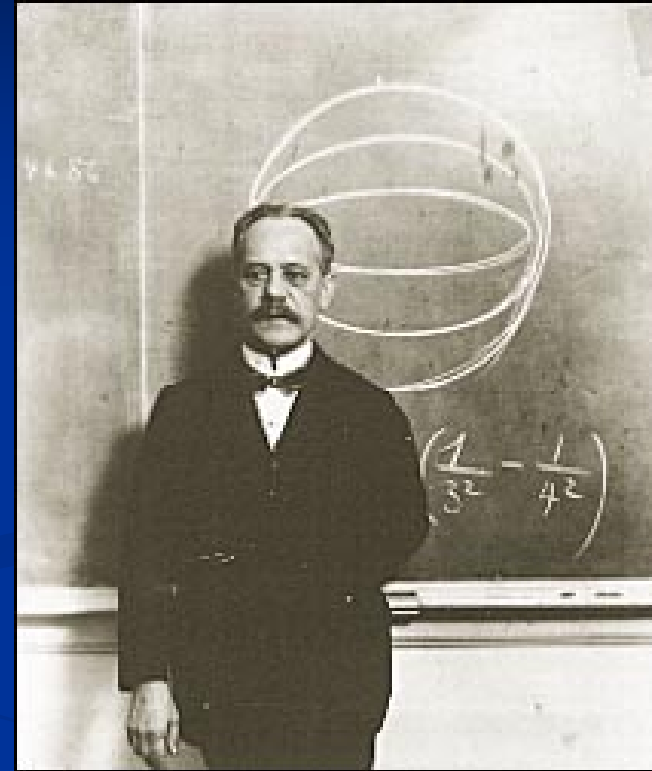
Image: en.wikipedia.org

- Worked as an assistant to Arnold Sommerfeld (Munich 1913-1921)
- Proposed the “octet rule” independently of G.N.Lewis (1916)
- Explained factor $(Z-1)$ in Moseley’s Law attributable to the shielding of charge due to the remaining “inner-shell” electron; factor of $3cR/4$ from Bohr’s theory.
- Developed the Sommerfeld-Kossel displacement law; identifying electronic similarities in isoelectronic species, C, N^+ , O^{2+}

Bohr-Sommerfeld Theory

Arnold Sommerfeld generalized Bohr's quantized orbits to conform to Albert Einstein's Special Theory of Relativity (1915); *fine structure* of X-ray lines.

- *“I do not think that I have ever enjoyed the reading of anything more than I enjoyed the study of them”, Bohr on Sommerfeld's theory of fine-structure (March 1916).*
- *“Your investigation of the spectra belongs among my most beautiful experiences in physics. Only through it do Bohr's ideas become completely convincing. If I only knew, what little bolts the Lord had used for it!” , Einstein on Sommerfeld's theory of atomic fine-structure (August 1916)*



Arnold Sommerfeld ca 1930

Image: <http://www.aip.org>

Bohr-Sommerfeld Theory

Relativistic classical mechanics, Bohr quantization, elliptical orbits

$$E = m_0 c^2 \left(1 + \frac{\alpha^2 Z^2}{\left(n_r + \sqrt{n_\phi^2 - \alpha^2 Z^2} \right)^2} \right)^{-1/2} = M c^2$$

n_r and n_ϕ are integers, α is the fine-structure constant and $M < m_0$.

For the $1s_{1/2}$ ground-state energy, we find (after some algebra) that

$$E = m_0 c^2 - \frac{m_0 e^4}{8 \epsilon_0^2 h^2} Z^2 - \frac{m_0 e^8}{128 \epsilon_0^4 h^4} \frac{Z^4}{c^2} - \dots$$

Rest-mass
energy

Non-
relativistic
Bohr energy

Relativistic
corrections

Quantum Mechanics 1925-1928

$$H\Psi = E\Psi$$

- Bohr orbits replaced by a wavefunction, Ψ , solution of the Schrödinger equation and the “Copenhagen interpretation” of $|\Psi|^2$ as a probability distribution.
- The energies, E , are *exactly* the same as those obtained by Bohr’s Theory.
- Dirac merged quantum mechanics and electrodynamics to obtain a more satisfactory description of absorption and emission of radiation, compared with Bohr-Sommerfeld theory.
- Pauli Exclusion Principle for fermions and the *Aufbau Prinzip* explained the valence structure of the elements.

Dirac Equation (1928)

- Dirac extended quantum mechanics to include special relativity
- Electron spin was a natural consequence of the relativity principle.
- C.G. Darwin showed that the solutions of the Dirac equation for an electron in a Coulomb field corresponded *exactly* to the energies in the Bohr-Sommerfeld fine-structure formula

Dirac Equation (1928)

$$E = \pm m_e c^2 \sqrt{1 + \left(\frac{p}{m_e c}\right)^2} = \pm M c^2$$

This is the relativistic energy of a free electron of momentum p , both classically *and* quantum mechanically.

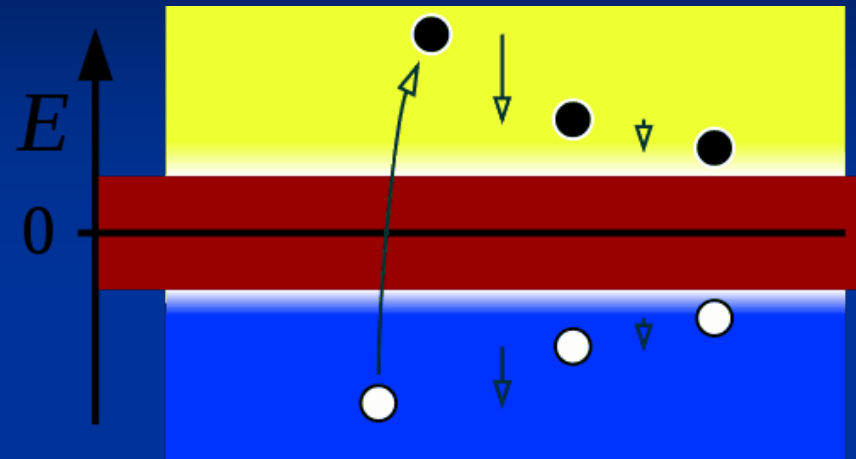
Classically, one chooses the + sign and rejects the – sign as unphysical.

Quantum mechanically, there is no basis to reject the – sign.

Just like X-ray spectra, all matter should decay radiatively from a positive energy state to a negative energy state.

Dirac Equation (1928)

Dirac solved the problem of negative energy states by invoking principles of X-ray spectroscopy.



- Negative-energy states filled in vacuum using Pauli Principle; subtract this (infinite) vacuum energy at end.
- Create a hole in the “negative energy sea” and the hole (white) behaves like an electron (black) with a positive charge (positron). The electron-positron pair annihilates radiatively.
- This model predicted the discovery of the positron by Anderson in 1932 and led to the development of *quantum field theory*.

Dirac's Edict

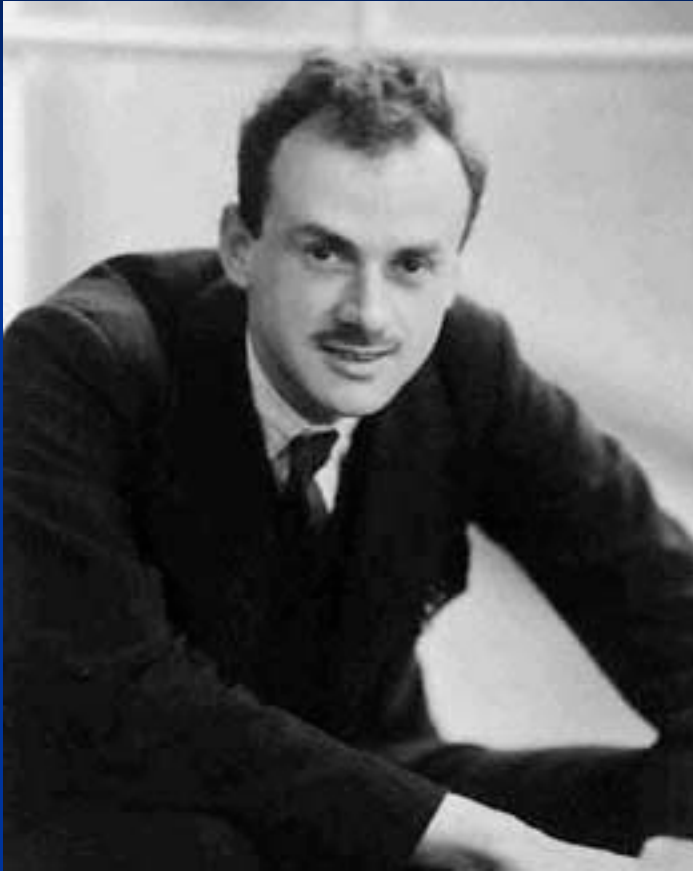


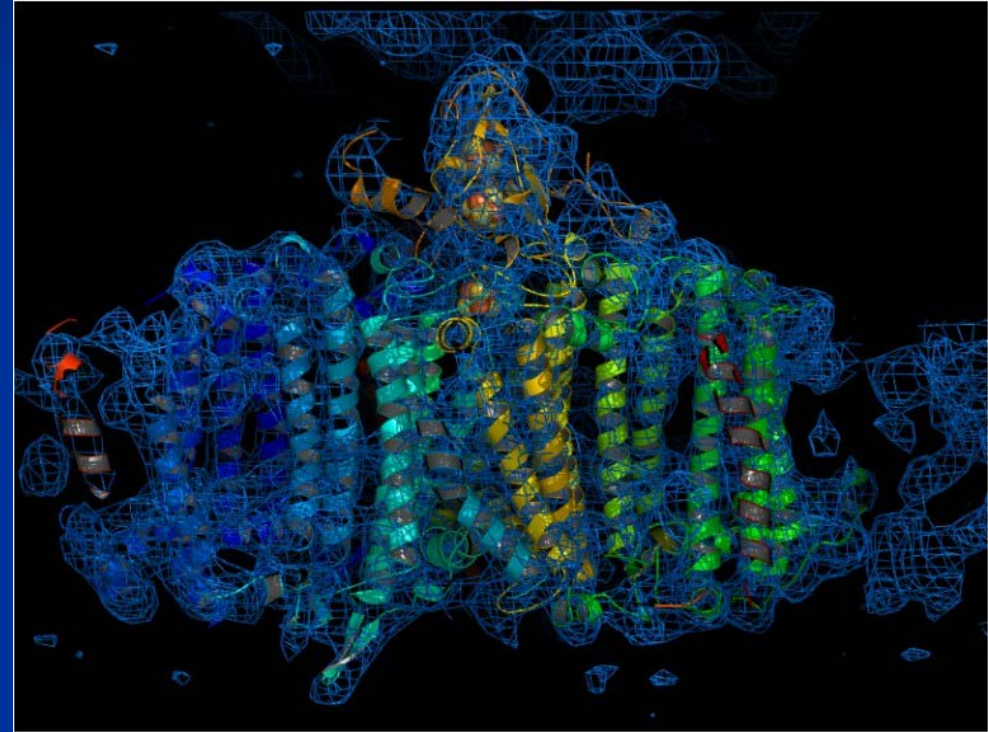
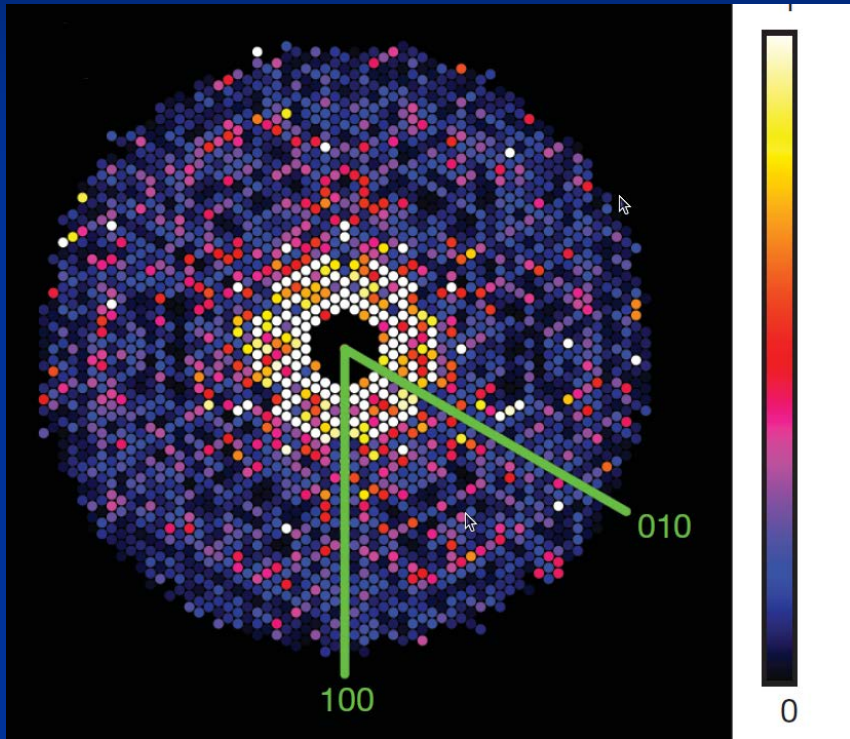
Image: Cavendish Laboratory, 1930

“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known...

...lead to an explanation of the main features of complex atomic systems without too much computation”.


P.A.M. Dirac, Proceedings of the Royal Society, A123, 792 (1929)

Part III: X-ray Scattering and the structure of materials and biomolecules



Diffraction and molecular structure of photosystem I using XFEL illumination, H. N. Chapman et al., *Nature*, **470**, 73-76 (2011).



The Third Revolution



MASSACHUSETTS INSTITUTE OF TECHNOLOGY

The Third Revolution:

The Convergence of
the **Life Sciences**,
Physical Sciences,
and **Engineering**



The Third Revolution

MIT White Paper (January 2011) outlines policies for encouraging innovation in Life Sciences; embedding successful interdisciplinary research within programs of the National Institutes of Health. Three “revolutions” are identified:

- 1. Molecular and Cell Biology (1953): understanding of cells and diseases; genetic engineering.
- 2. Genomics (1985): understanding an entire genome: basic DNA sequence, location of genes, intragenomic phenomena. Driven by availability of supercomputational resources.
- 3. Convergence (2005): merging of physical, engineering and life sciences for the mutual benefit of all, but especially biomedical research.

Revolution Zero: Hooke's Micrographia (1665)

MICROGRAPHIA:
OR SOME
Physiological Descriptions
OF
MINUTE BODIES
MADE BY
MAGNIFYING GLASSES
WITH
OBSERVATIONS and INQUIRIES thereupon.

By *R. HOOKE*, Fellow of the **ROYAL SOCIETY**.

*Non possi oculo quantum contendere Linceus,
Non tamen idcirco contemnas Lippus: utorgi. Horac. Ep. lib. 1.*



LONDON, Printed by *Jo. Martyn*, and *Ja. Allestry*, Printers to the
ROYAL SOCIETY, and are to be sold at their Shop at the *Bell* in
S. Paul's Church-yard. M DC LX V.

MICROGRAPHIA RESTAURATA:
OR, THE
COPPER-PLATES
OF
Dr. *HOOKE*'s Wonderful Discoveries
BY THE
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Whereby the most Valuable PARTICULARS in that

Celebrated **AUTHOR**'s

MICROGRAPHIA

Are brought together in a narrow Compass;

AND

Intermixed, occasionally, with many Entertaining and Instructive DISCOVERIES and OBSERVATIONS in **NATURAL HISTORY**.

Rerum Natura nequam magis quàm in minimis tota est.
PLIN. Hist. Nat. Lib. XI. C. 2.

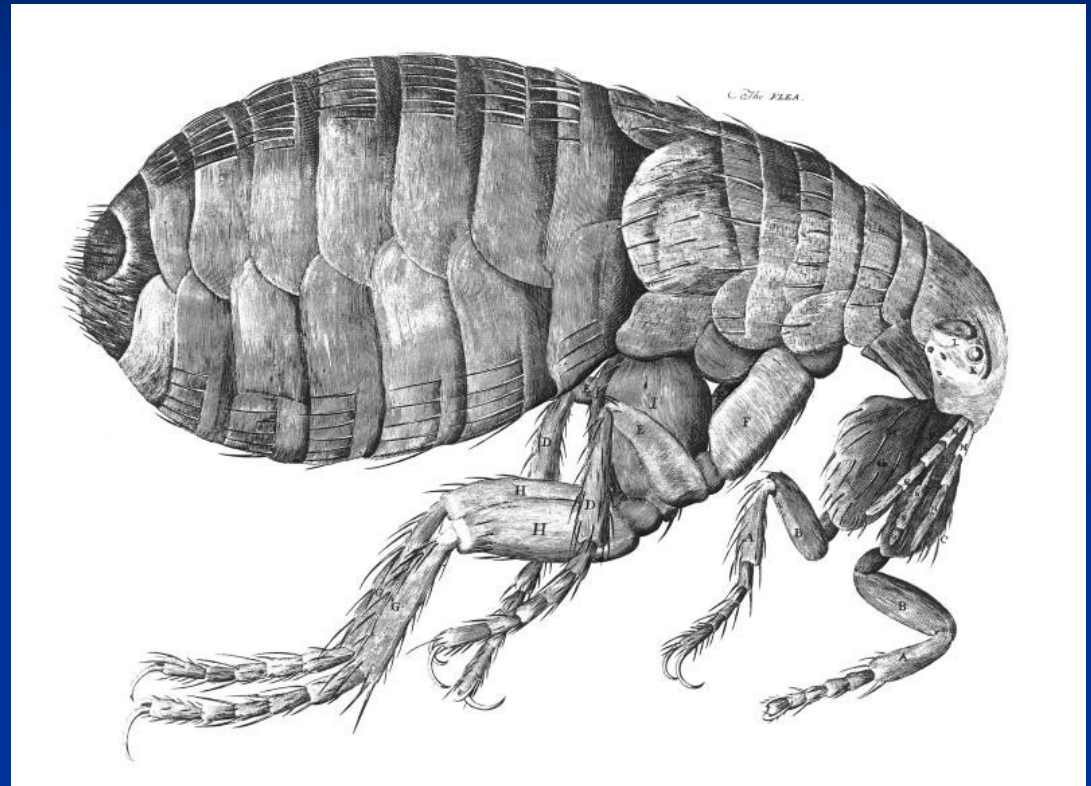
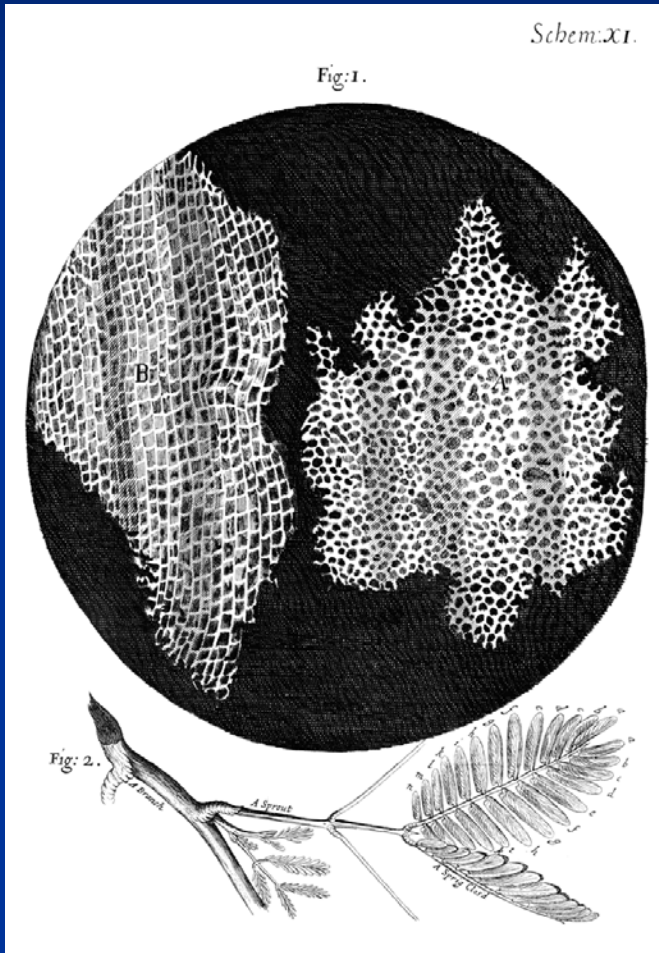


LONDON:

Printed for and Sold by **JOHN BOWLES**, Printseller at the *Black Horse* in *Cornhill*.
Sold also by **R. DODDSTEV**, in *Patnall*, and **JOHN CURT**, Optician, in *Fleetstreet*.

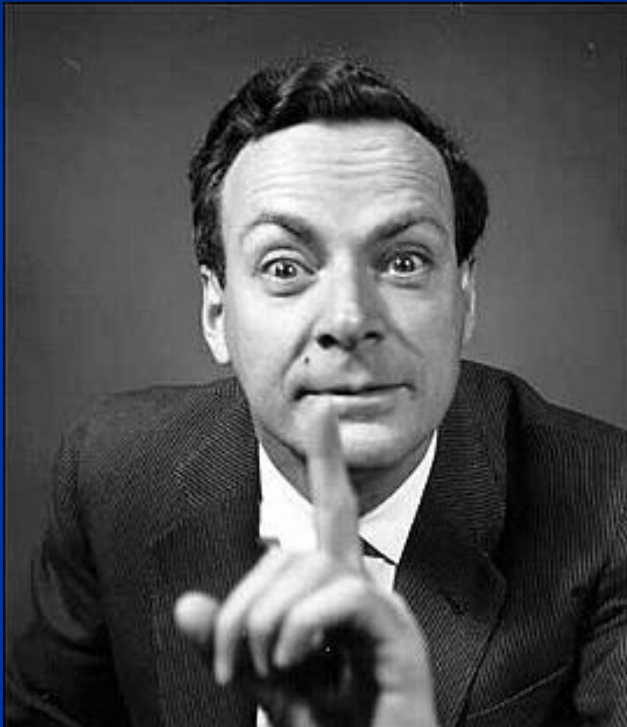
MDCCLXV.

Revolution Zero: Hooke's Micrographia (1665)



Images: Micrographia, R Hooke, 1665.

Revolution Zero: There's Plenty of Room at the Bottom", R. P. Feynman (1959).

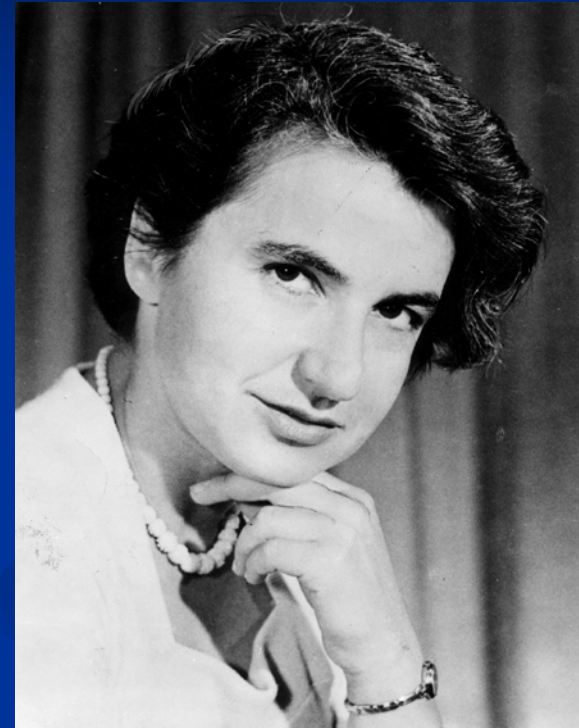
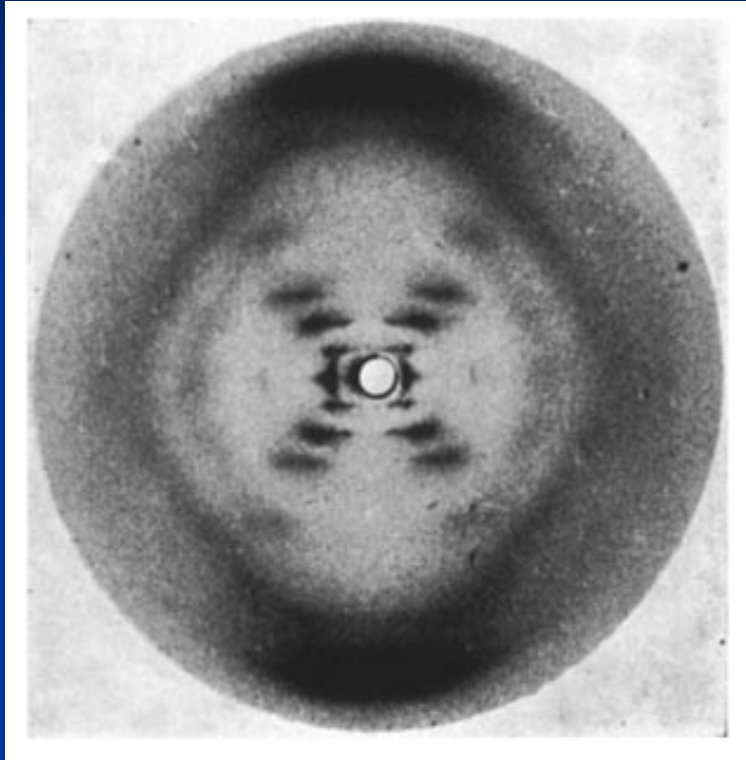


Feynman on biology: the way to answer most fundamental questions in biology is: you just look at the thing! (microscopy).

Feynman on information: there is no fundamental prohibition to the manipulation of matter and the encoding of information at the atomic level (nanotechnology).

The *molecular microscope* is the logical outcome of developing “better microscopes” for biology. One imagines that Hooke would agree.

Revolution 1: Protein Crystallography

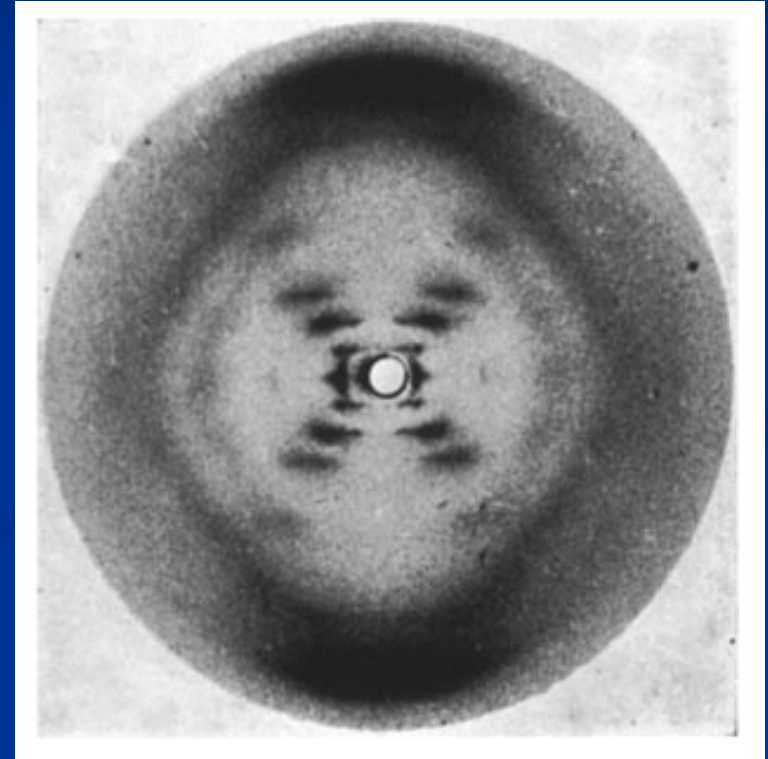


Rosalind Franklin obtained the diffraction pattern of a 'damp' crystalline sample of DNA in 1952. This image is now known as 'Photo 51'. It is one of the most famous and important images in science. Ever.

Revolution 1: Protein Crystallography

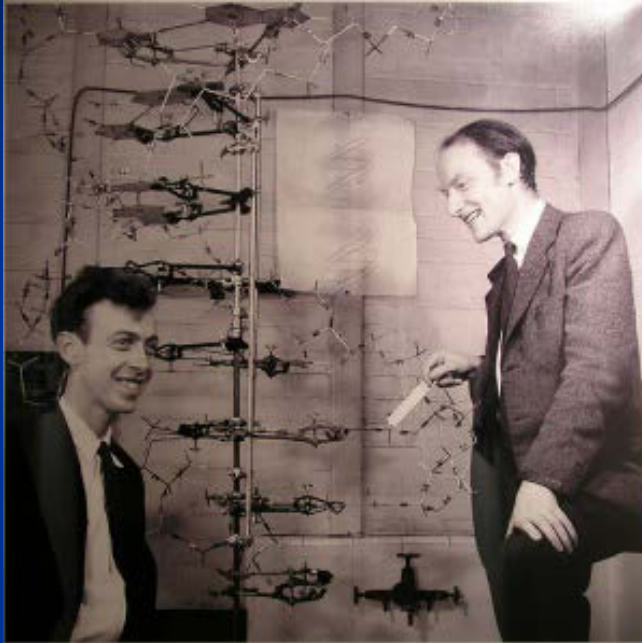
What does Photo 51 "mean"?

- The cross is characteristic of a helical structure(s).
- The distance between the dark spots on the cross indicates that the helices repeat every 34 angstrom.
- The distance from the centre to the edge indicates that the distance between "rungs" is 3.4 angstrom (ten rungs per helix unit)
- The "double helix" structure is required by "Chargall's Principle". The amount of cytosine and guanine must be identical, and the amount of thiamine and adenine must be identical. Only possible if the structure is two opposed (interlinked) helices, with C-G and T-A pairing.



This double helix structure is *the blueprint of life.*

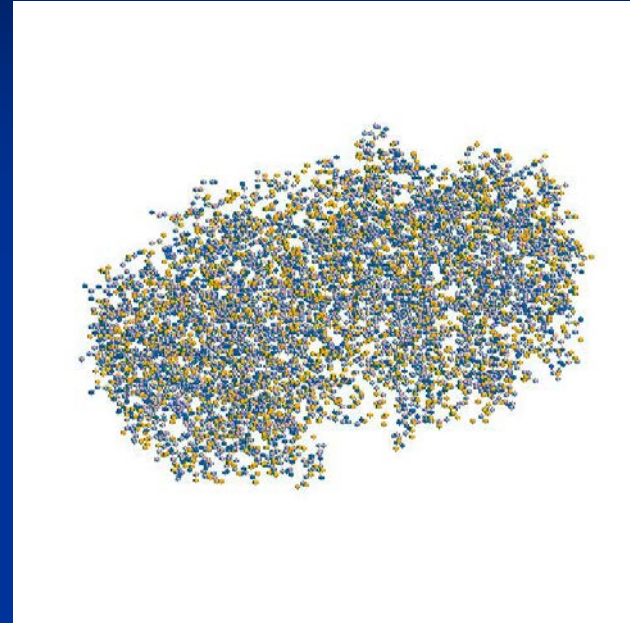
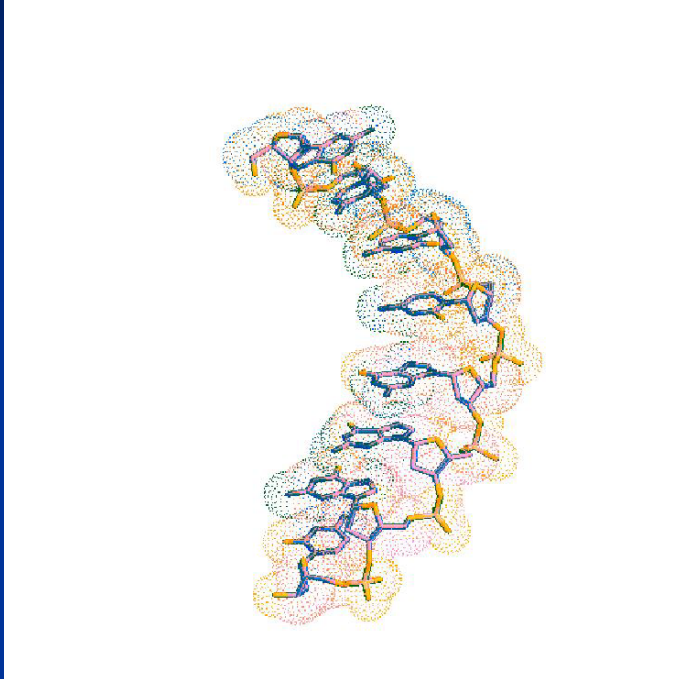
Revolution 1: Protein Crystallography



Crick and Watson (1953), and the DNA "meccano model". This model was made with old bits of wire and tin and bunsen burner clamps.

It is now on display in the London Science Museum.

Revolution 1: Applications



Molecular structures of DNA (left) and the influenza virus (right). The structure of influenza was used by CSIRO to develop the anti-viral medicine, *Relenza*.

The H5N1 virus has the potential to decimate the human population: Relenza is the most effective treatment

Revolution 1: applications

- Imaging of materials, including biological materials, with sub-nanometre (atomic) resolution
- Molecular structure determination of individual molecules, or small clusters of molecules, without the need to grow high-quality crystals.
- The potential of this approach to solving problems in structural biology (molecular biology, pharmacology) and to health, veterinary and agricultural technologies is huge.
- CXS develops methods towards the aim of determining the molecular structure of non-crystalline samples of membrane proteins.

Revolution 2: Genomics

Genomics: sequence, assemble and analyze the function and structure of genomes (complete set of DNA in a single cell of an organism)



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Cray T3E: Daresbury Laboratory, UK, 1998

IBM Blue Gene/Q: Victorian Life Sciences Computation Initiative, UoM (2012)

http://tardis.dl.ac.uk/computing_history.

Revolution 3: Convergence

Large-scale interdisciplinary programs applying the tools and expertise of fundamental physics to problems in the life sciences.

Utilize large, international research facilities:

Supercomputers, synchrotron, free-electron laser, electron microscope, particle accelerator

...whatever and whoever it takes to get the job done.

Microscopes: 1665-2013



Leica Super-resolution confocal microscope (Leica TCS SP8 STED), 2007

Hooke's optical microscope, 1665

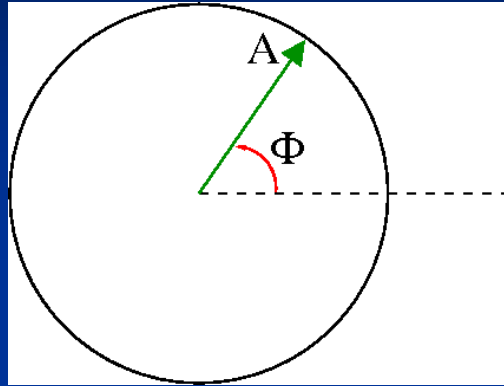
Images were illuminated by stabilized laser illumination of femtosecond pulses, producing X-ray photons in 10^{-15} s. California, USA, reproduction

computational processing of data

Linac Coherent Light Source (LCLS), 2009

Beamline scientists and engineers, experimental and theoretical physicists, structural biologists and computer analysts work together.

Coherent Light Sources



The properties of light (including X-rays) depend primarily on two quantities:

1. Amplitude, A . Absorption causes A to decrease.
2. Phase, Φ . The phase increases as light travels from point to point, at a rate that depends on frequency and the medium through which it travels.

Photographs record intensity, $I = A^2$; information about Φ is lost.

Coherent Light Sources

- A beam of fully-coherent light is one for which we know the relationship Φ between I everywhere in the beam. It's always easy to measure I , but hard to measure Φ , especially for X-rays.
- Lasers are examples of fully-coherent light sources.
- Synchrotrons produce light with 'partial' (not quite full) coherence.
- X-ray Free-electron lasers have high spatial and temporal coherence
- Thermal sources (incandescent lights) are called 'incoherent'.
- The phase of the light changes when it passes through a material, or encounters an obstacle, compared to what happens to Φ in free space; diffraction. That change in Φ carries information about the material.

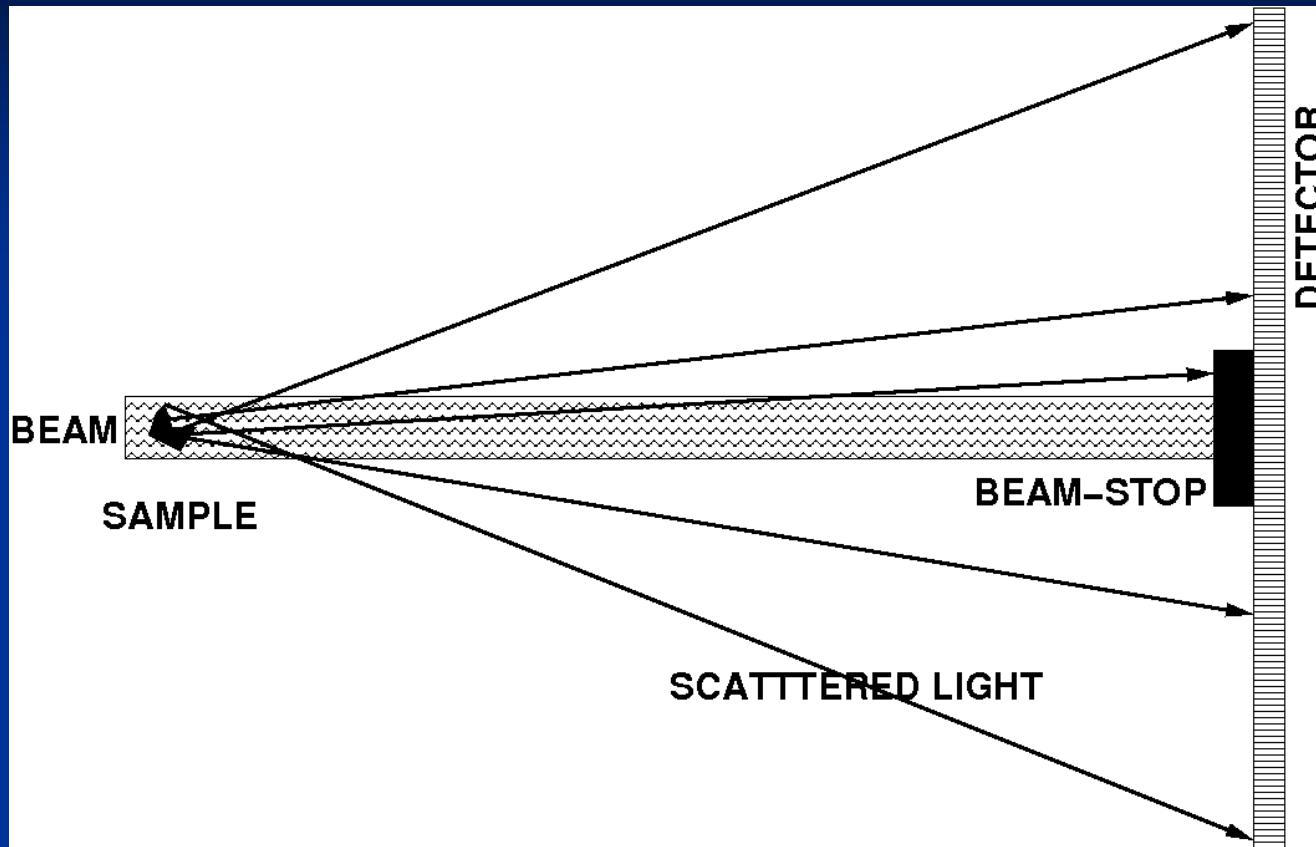
Coherent X-ray Light Sources

Australian Synchrotron,
Melbourne



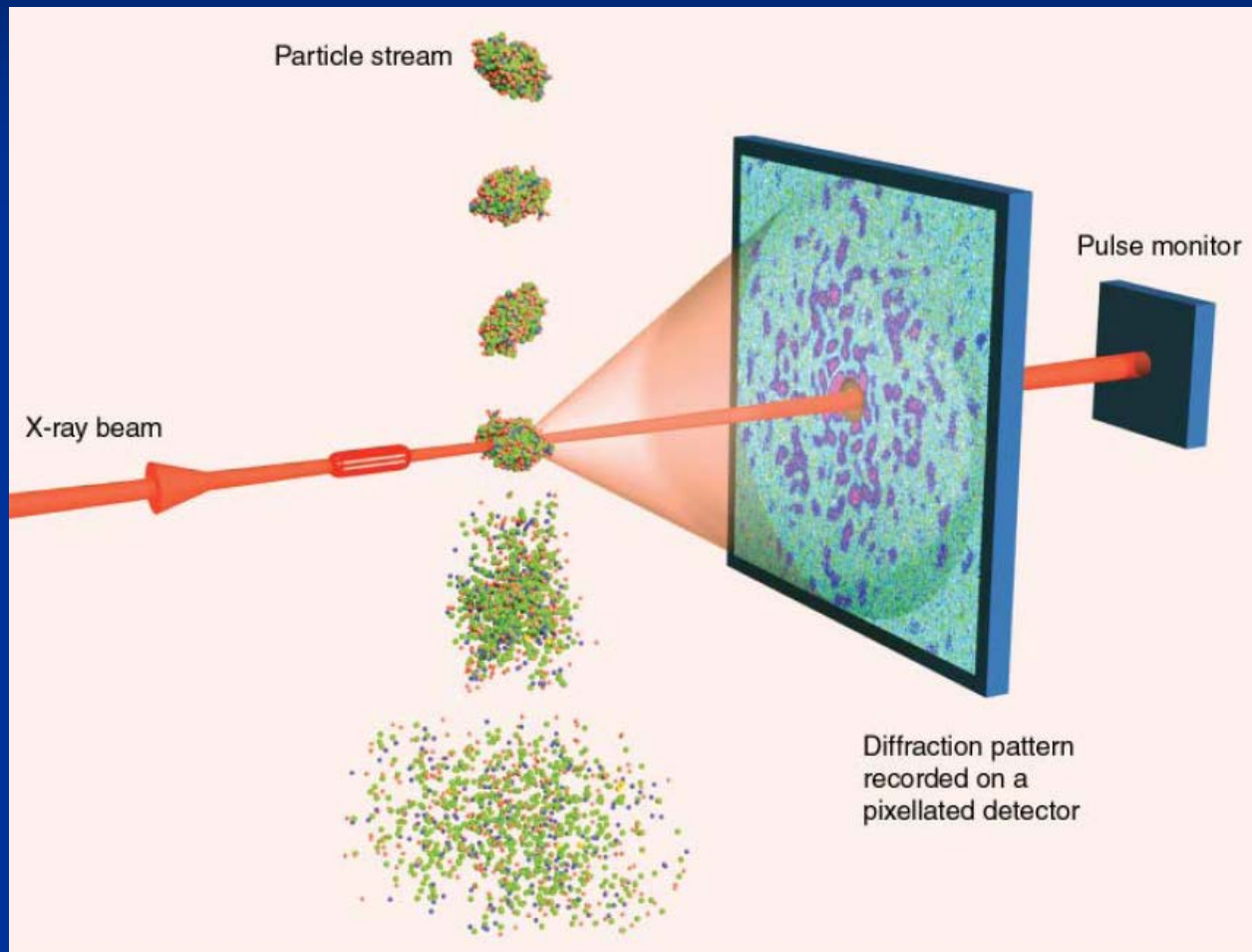
X-ray free-electron laser, LCLS USA

What is diffraction?

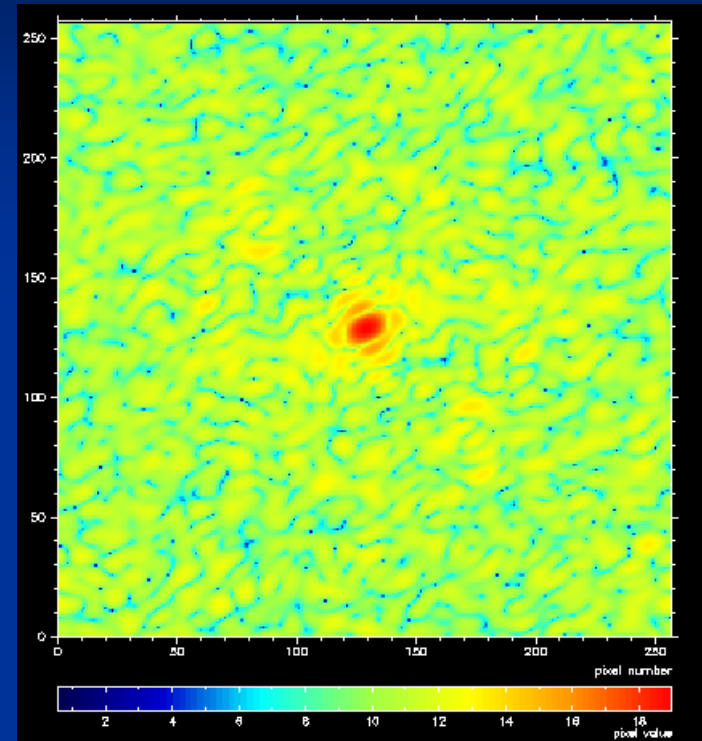
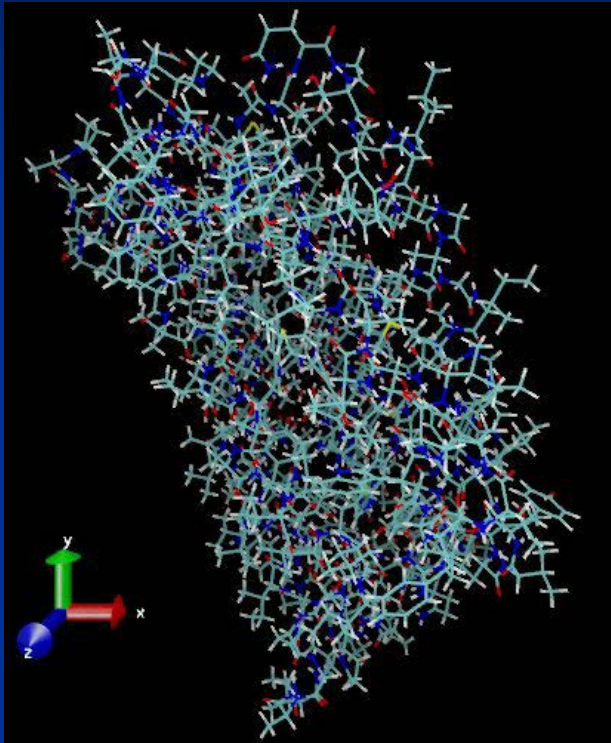


Schematic diagram of diffraction using an intense light source. You can only measure the intensity using a detector (it's just a photograph)

Diffract and Destroy imaging: the molecular X-ray microscope



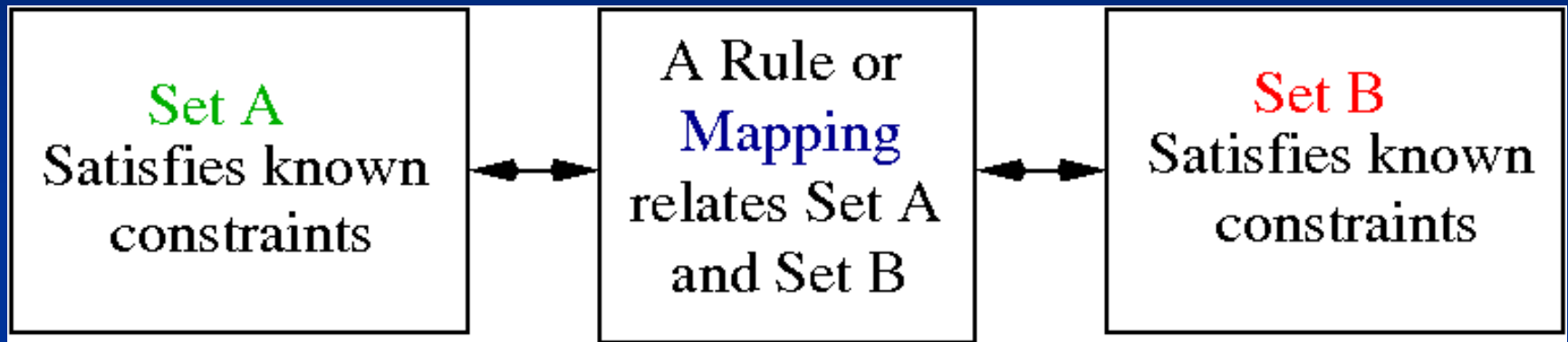
Diffraction imaging of single molecules



Simulated X-ray diffraction pattern (left) generated by a single bacteriorhodopsin molecule (model, right).

If we could solve this physics problem, it would *revolutionize* structural biology; no need for crystallization.

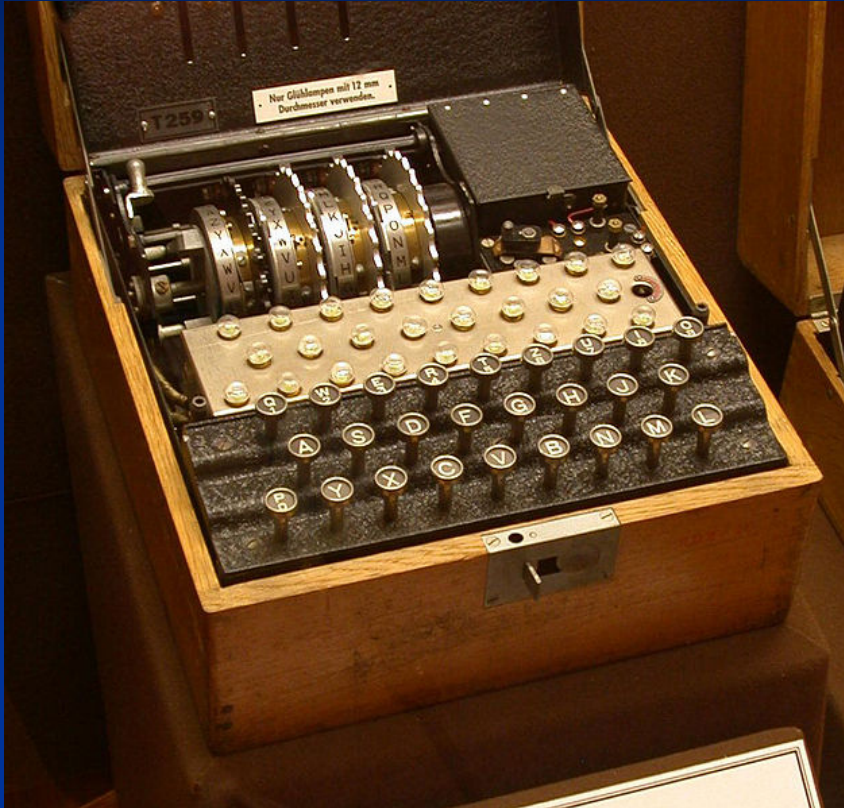
The molecular structure problem is closely related to Sudoku puzzles and code-breaking



Sudoku problems, the coherent diffractive imaging problem and breaking the Enigma code can all be solved by thinking about them in the above way.

Although they are *physically* dissimilar, they can be put into a *mathematically* equivalent form (constrained projections).

The Enigma Code



- Set A: the original message "*nichts zu melden*"
- Set B: the encoded message, XFTRG GHTFR SWEDF
- mapping: a machine whose initial settings for each message were changed every day (many downloadable simulators).

By running through the possible settings on the first few letters, the Allies could read *every* coded message for that day: a little information revealed the mapping.

The weakness was human habit: there was one operator who was known always to transmit *nichts zu melden* (nothing to report) each morning.

Extracting molecular structure from continuous X-ray diffraction data

Technically speaking, this involves “the solution of a mathematical inverse problem using *a priori* information by the method of iterated projections”



Sir Ernest Rutherford: *“If you can't explain your physics to a barmaid it is probably not very good”*

...it would be even better if we could explain it to high school students!

Growing Tall Poppies: a student outreach program



Dr Eroia Barone-Nugent, science teacher, Santa Maria College Northcote, developer of the program Growing Tall Poppies: an authentic experience in science

Sudoku : some assembly required



Of course one can write an iPhone app to do this, but instead we revived some of the spirit of Crick and Watson and make a simple device to help us solve Sudoku puzzles. It's not very elaborate, but it does the job.

It's a board game.

1	2	3	1	2	3	1	2	3
4	5	6	4	5	6	4	5	6
7	8	9	7	8	9	7	8	9
1	2	3	1	2	3	1	2	3
4	5	6	4	5	6	4	5	6
7	8	9	7	8	9	7	8	9
1	2	3	1	2	3	1	2	3
4	5	6	4	5	6	4	5	6
7	8	9	7	8	9	7	8	9

Impose the constraint on each 3x3 block by colouring the tiles. *Any* valid Sudoku can be generated by permuting tiles of the same colour to satisfy row and column constraints.

Any permutation of the 3x3 blocks can be obtained by a series of pairwise tile swaps.

1	9	2	4	7	3	9	2	3
6	4	3	2	5	9	5	8	6
5	8	7	1	6	8	7	4	1
4	1	5	5	3	4	4	8	3
3	2	9	7	2	6	1	9	5
7	6	8	1	8	9	7	2	6
7	2	1	2	8	1	3	4	9
8	6	9	4	5	6	1	5	6
4	3	5	3	9	7	2	7	8

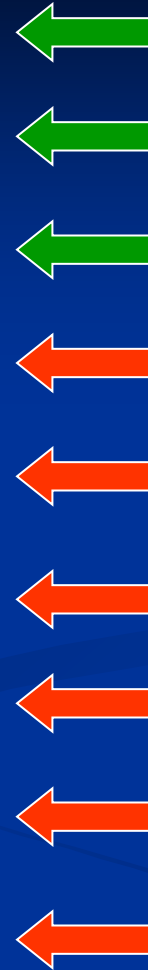


Initialize the procedure with the *fixed* clue tiles (white reverse side) as constraints.

The remaining coloured tiles are assigned randomly to each 3x3 block

The only valid move is to swap tiles of the same colour.

6	9	2	4	7	8	5	1	3
1	4	3	2	5	9	7	8	6
5	8	7	1	6	3	2	4	9
4	1	5	5	3	4	4	8	3
3	2	9	7	2	6	1	9	5
7	6	8	1	8	9	7	2	6
7	2	1	2	8	1	3	4	9
8	6	9	4	5	6	1	5	6
4	3	5	3	9	7	2	7	8



The row constraint is next satisfied for each group of three only by sequential tile swaps of the same colour

6	9	2	4	7	8	5	1	3
1	4	3	2	5	9	7	8	6
5	8	7	1	6	3	2	4	9
6	1	9	5	8	2	4	7	3
3	2	4	7	1	6	8	9	5
5	7	8	4	3	9	1	2	6
7	2	1	2	8	1	3	4	9
8	6	9	4	5	6	1	5	6
4	3	5	3	9	7	2	7	8



Don't worry about the columns! Just fix the rows by applying like colour tile swaps

6	9	2	4	7	8	5	1	3
1	4	3	2	5	9	7	8	6
5	8	7	1	6	3	2	4	9
6	1	9	5	8	2	4	7	3
3	2	4	7	1	6	8	9	5
5	7	8	4	3	9	1	2	6
7	2	5	4	8	1	3	6	9
8	6	9	3	7	2	1	5	4
4	1	3	5	9	6	2	7	8



All row constraints are now satisfied.

6	9	2	4	7	8	5	1	3
1	4	3	2	5	9	7	8	6
5	8	7	1	6	3	2	4	9
9	1	6	5	8	2	4	7	3
3	2	4	7	1	6	8	9	5
7	5	8	4	3	9	1	2	6
2	7	5	4	8	1	3	6	9
8	6	9	3	7	2	1	5	4
4	3	1	5	9	6	2	7	8



Now satisfy the constraints for the columns by performing only swaps of the same colour

6	9	2	8	7	4	5	1	3
1	4	3	9	5	2	7	8	6
5	8	7	1	6	3	2	4	9
9	1	6	5	2	8	4	7	3
3	2	4	7	1	6	8	9	5
7	5	8	3	4	9	1	2	6
2	7	5	4	8	1	3	6	9
8	6	9	2	3	7	1	5	4
4	3	1	6	9	5	2	7	8



6	9	2	8	7	4	5	1	3
1	4	3	9	5	2	7	8	6
5	8	7	1	6	3	9	4	2
9	1	6	5	2	8	4	3	7
3	2	4	7	1	6	8	9	5
7	5	8	3	4	9	6	2	1
2	7	5	4	8	1	3	6	9
8	6	9	2	3	7	1	5	4
4	3	1	6	9	5	2	7	8



Solved!

*All constraints
are now
satisfied*

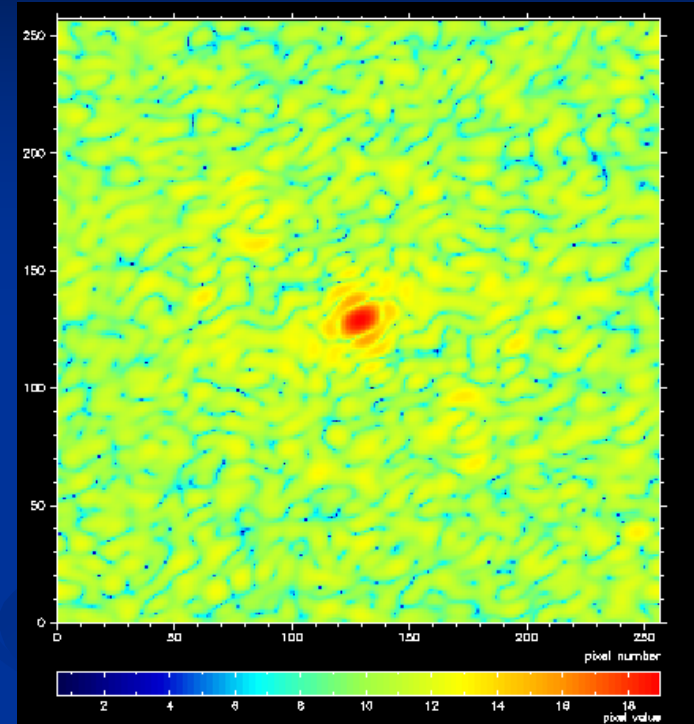
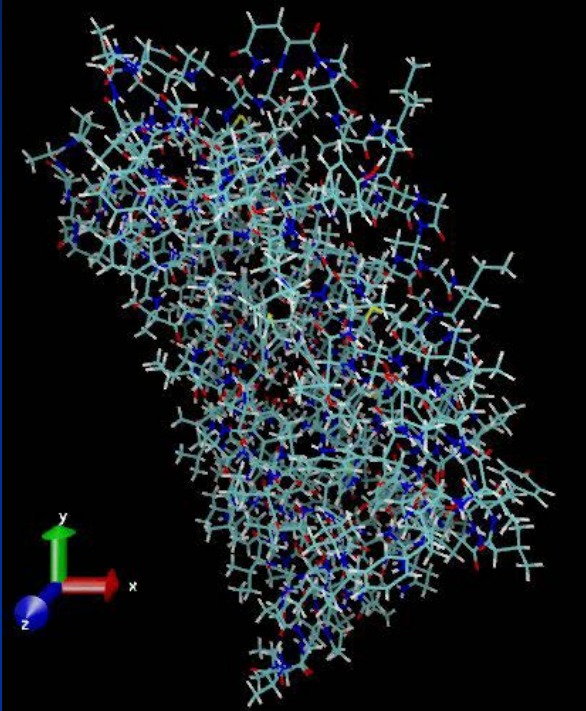
6	9	2	8	7	4	5	1	3
1	4	3	9	5	2	7	8	6
5	8	7	1	6	3	9	4	2
9	1	6	5	2	8	4	3	7
3	2	4	7	1	6	8	9	5
7	5	8	3	4	9	6	2	1
2	7	5	4	8	1	3	6	9
8	6	9	2	3	7	1	5	4
4	3	1	6	9	5	2	7	8



This was an easy
Sudoku. The
algorithm
terminated
because the
column
constraints
involved only
horizontal swaps

Generally, one
alternates
between rows
and columns
until a solution
is obtained; an
iterative,
projective
algorithm

Diffraction imaging of single molecules

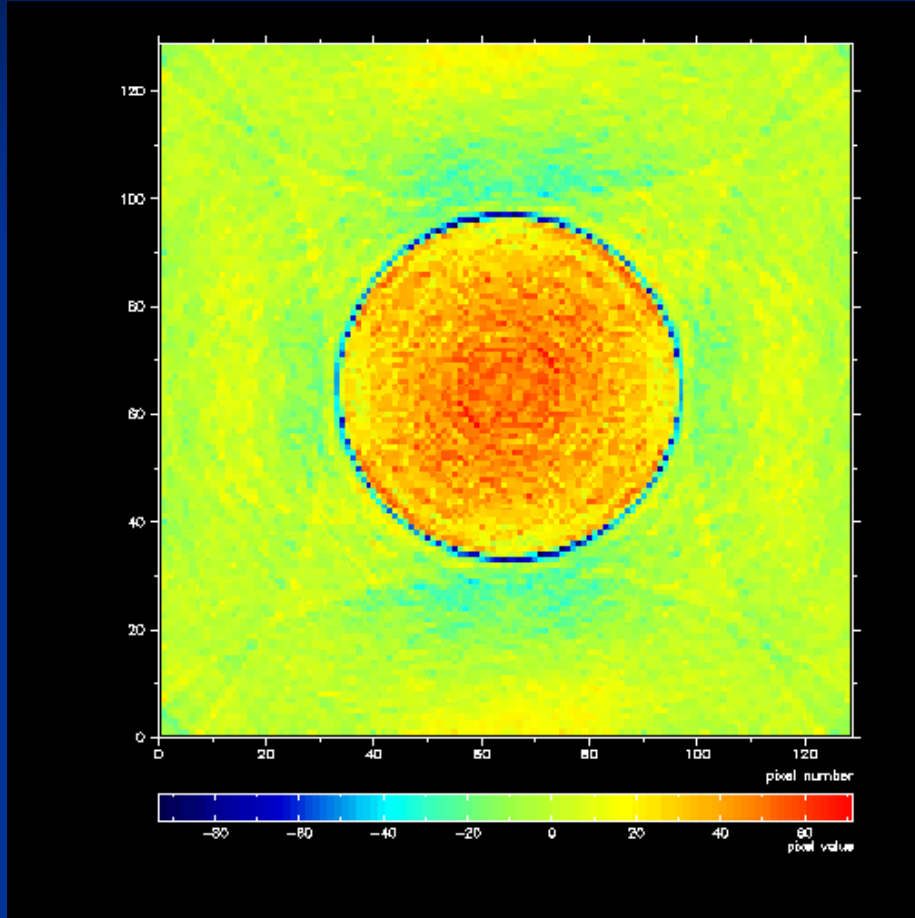


Constraint A: maximum size of molecule (finite support)

Constraint B: amplitude of the X-ray wave measured at the detector

Mapping: mathematical propagation of light between the molecule and the detector

Reconstruction of *bacteriorhodopsin*



The procedure is initialized by a uniform sphere of electronic charge.

H. M. Quiney and K. A. Nugent, *Nature Physics*, 7, 142-146 (2011).

Image is a two-dimensional projection through the three-dimensional electron density: 1 angstrom resolution in about 500 iterations.

XFEL Science Today



Prof. Henry Chapman

PhD UoM Physics 1990



Melbourne,
Deputy Vice-
Chancellor (Research)
La Trobe



ARC Centre of Excellence for
COHERENT X-RAY SCIENCE

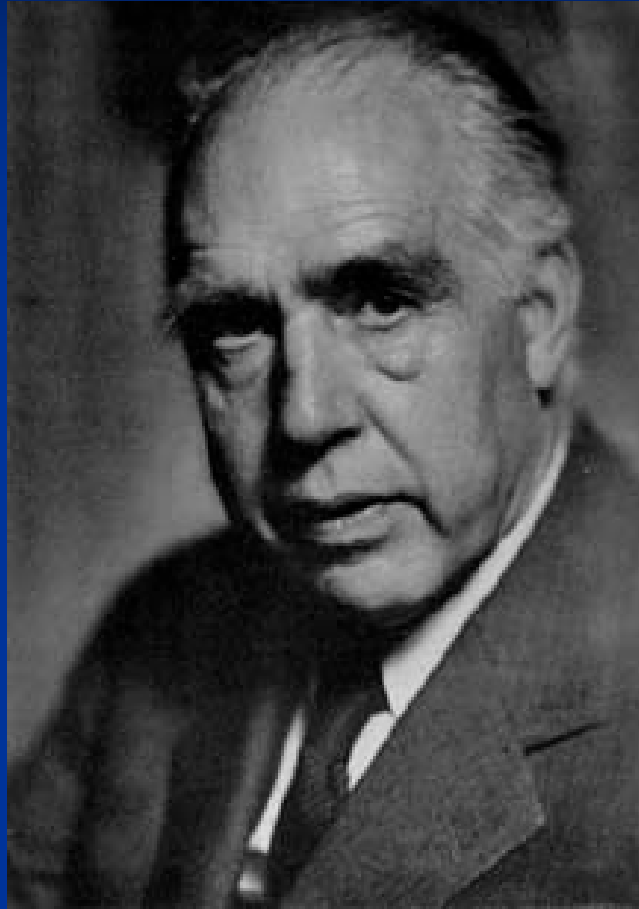


Director of CXS
2013-

Summary

1. Moseley was inspired by Bohr's theory to place the concept of atomic number on a firm basis, stimulating research into the nucleus, atomic structure, fine structure, chemistry and, ultimately, particle physics in the process.
2. X-ray scattering is the basis of crystallography and may, with the help of XFELs, be used to study dynamical processes in single molecules or clusters with atomic resolution in the life sciences.
3. Future research in physics and biology will be linked through collaborative, interdisciplinary projects involving international facilities: convergence.

A Parting Thought



“Everything we call real is made from things that cannot be regarded as real.

If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet”.

Niels Bohr 1885-1962