Early Days of X-ray Diffraction and The Birth of Dynamical Theory

André Authier
Université P. et M. Curie

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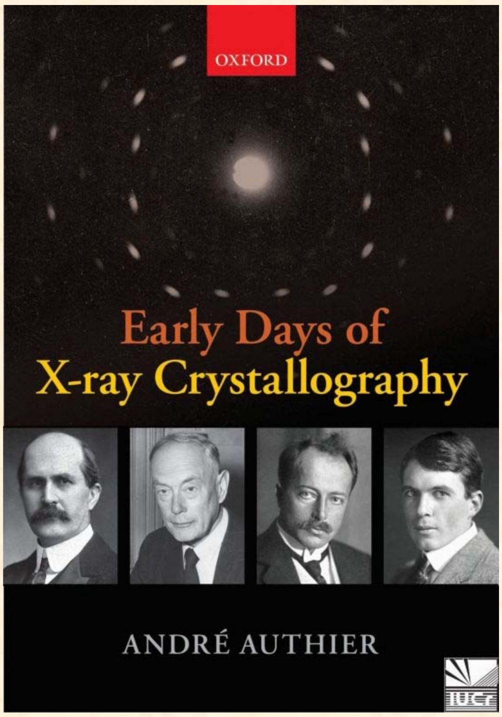

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The discovery of X-ray diffraction

1) Validated the space lattice hypothesis

2) Showed the wave nature of X-rays

3) Opened the route for the study of the

- Structure of the atom
- Atomic structure of solids
- Real structure of solids

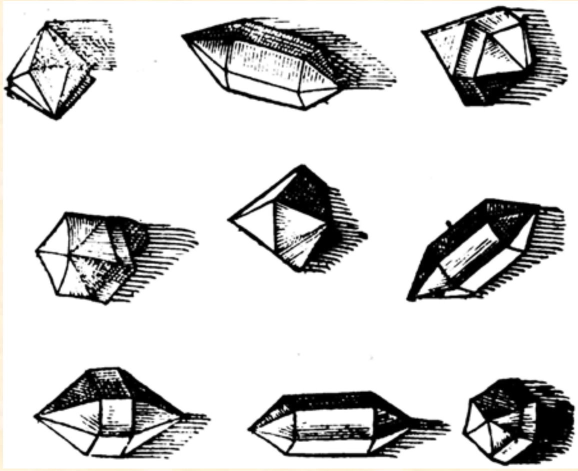
HOW DID THE CONCEPT OF SPACE LATTICE ARISE?

Crystalline nature of solid matter

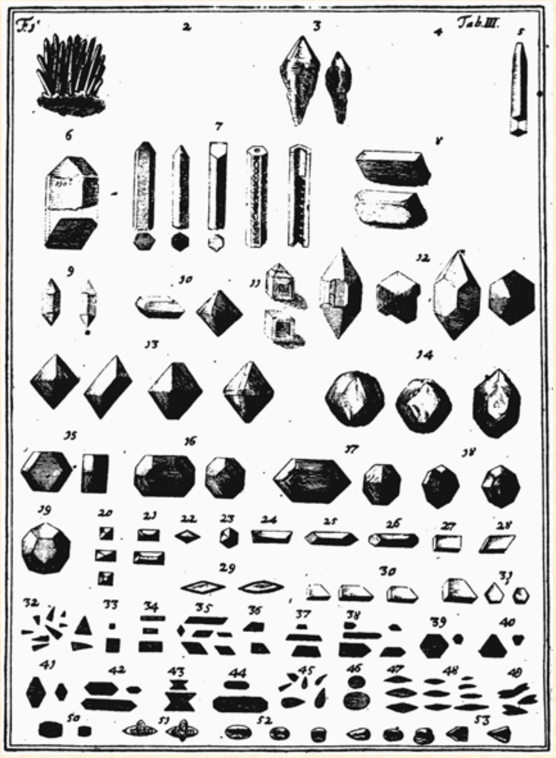
Crystal: greek Κρυσταλλοσ, latin **Crystallus** – ice
rock-crystal (quartz) due to the 'very strong congelation of water' (Aristotle, Pliny the elder → 16^{th} c. !)

Crystallography: Moritz Anton Cappeller (1685–1769) – in 1723
Podromus crystallographiae …

Crystals are polyhedral



Quartz crystals - Boece de Boot (1644)



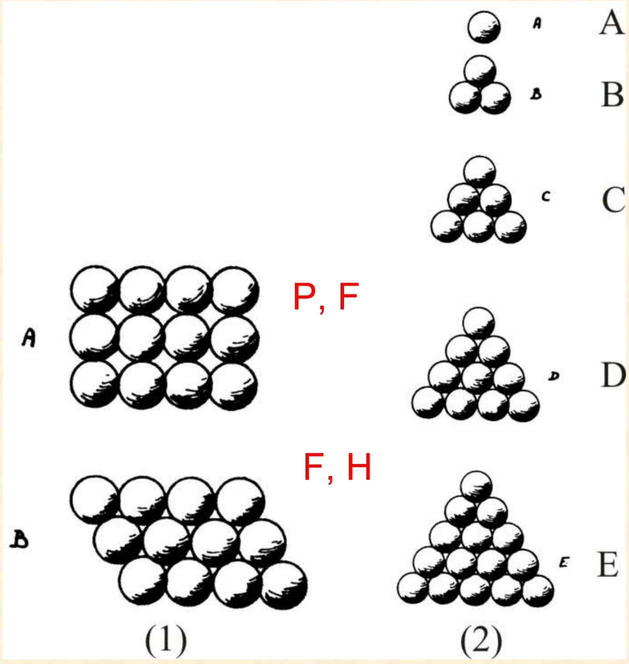
Crystal shapes. After Cappeller (1723)

The space lattice hypothesis – two theories:

- **Molecular theory**
  - ➢ Molecules or corpuscles exerting forces on one another, either polyhedral (space-filling approach) or spherical (close-packing approach)
- **Polar theory**
  - ➢ No ultimate atom, dynamic equilibrium of matter resulting from the action of forces centred at mathematical points, or poles, and oriented relative to the main cleage planes and growth faces

The close–packing approach

Johannes Kepler (1571 – 1630)



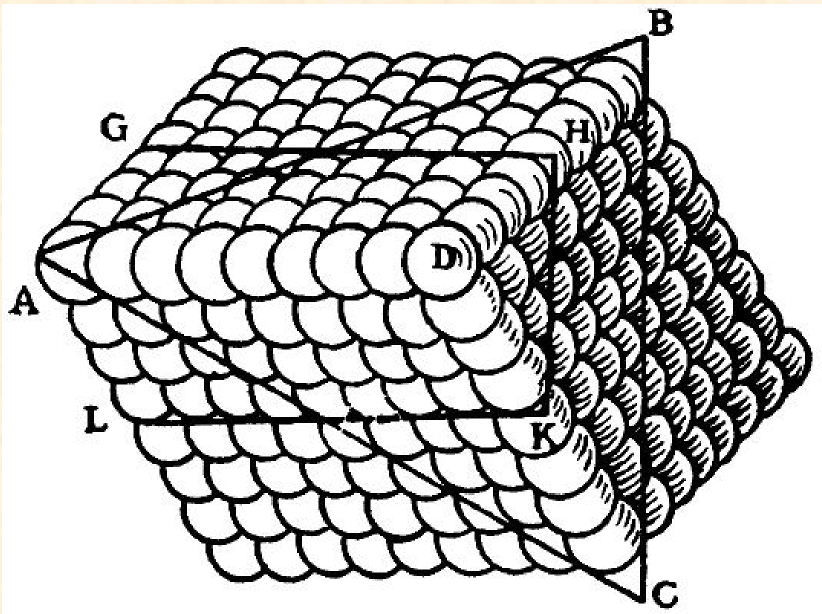
The six-cornered snowflake (1611)

The first pictures of space lattices: P, F, H

(M. von Laue – 1952)

The close–packing approach

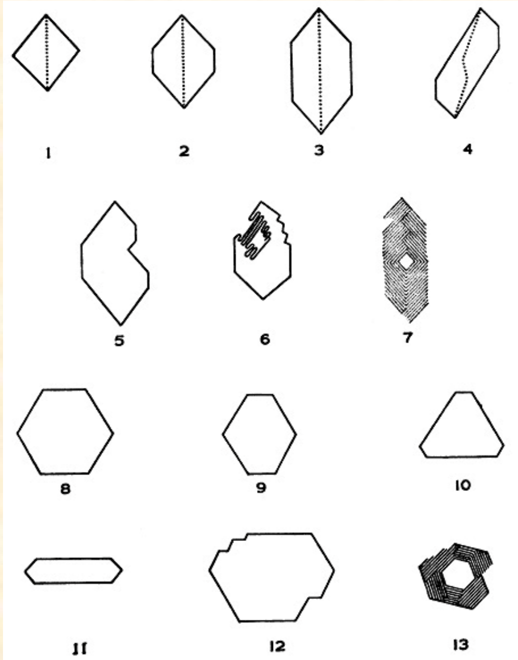
Christiaan Huygens
(1629-1695)



Structure of calcite ($CaCO_3$): a stacking of oblate ellipsoids – 1678

The constancy of interfacial angles

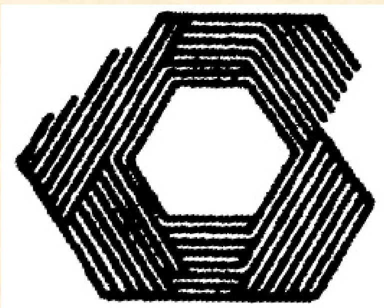
Nicolas Steno (1638 – 1686)



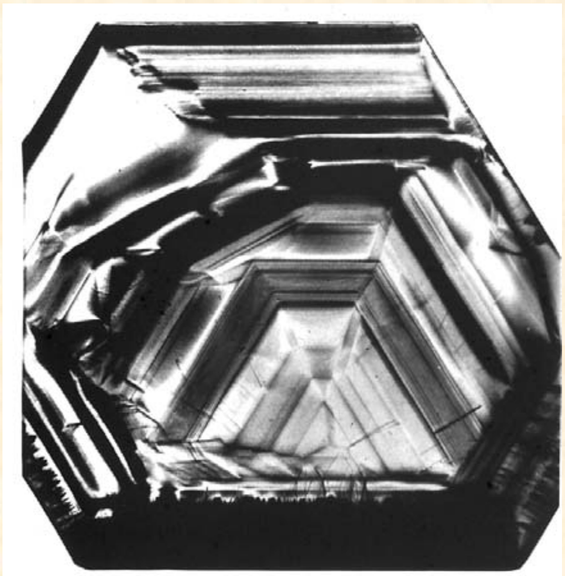
- Constancy of quartz interfacial angles
- Layer growth of crystals

Steno (1669)

Growth bands and sectors

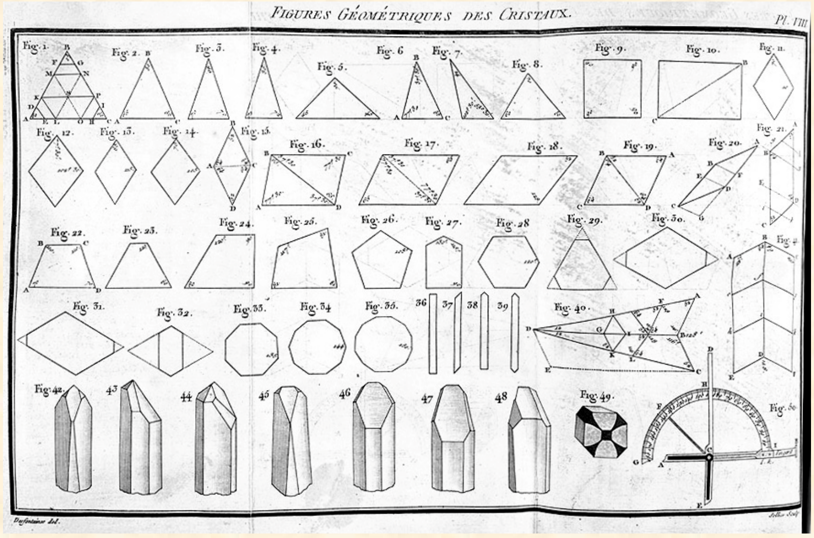


Steno (1669)



Actual topograph of a quartz crystal

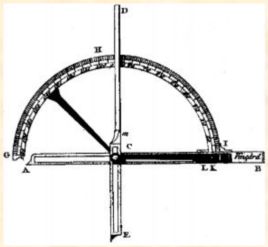
The constancy of interfacial angles



J.-B. Romé de l'Isle
(1736-1790)

Constancy of interfacial angles: generalization (1783)

A. Carangeot
(1742-1806)



The space–filling approach

Crystals are triperiodic assemblies of small blocks

Foundation of modern crystallography - R.-J. Haüy

The space–filling approach

Crystals are triperiodic assemblies of small blocks

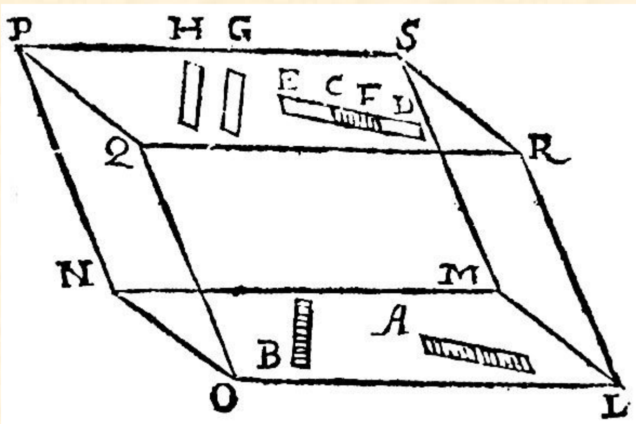
Cleavage of calcite

• R. Bartholin (1625-1698) – discovered of double refraction (1669)

The space–filling approach

Crystals are triperiodic assemblies of small blocks

Cleavage of calcite

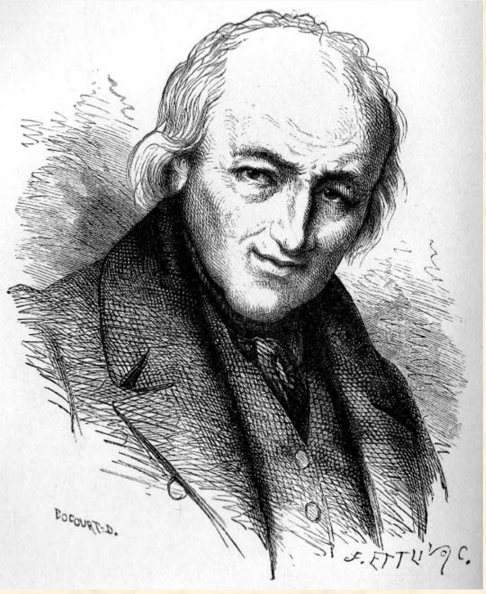


• R. Bartholin (1625-1698) – discovered of double refraction (1669)

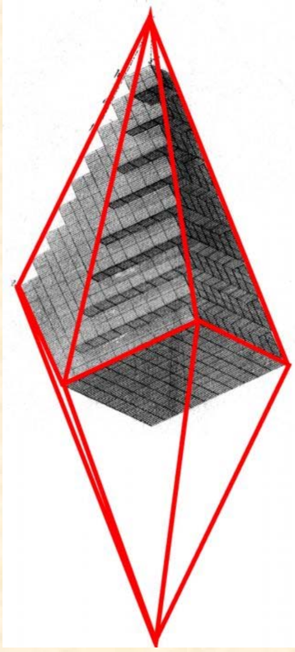
• C. Huygens (1629-1695) – explained double refraction (1678)

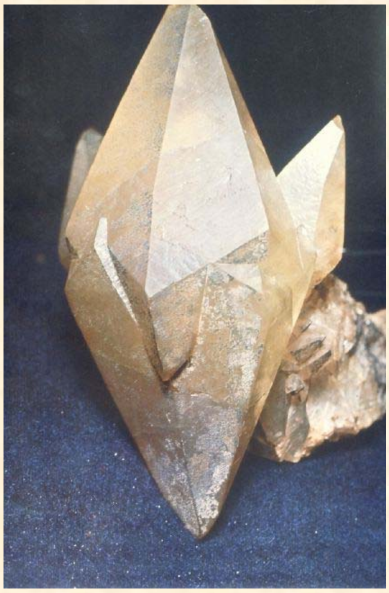
The space–filling approach

Crystals are triperiodic assemblies of small blocks



R.-J. Haüy (1743-1822)

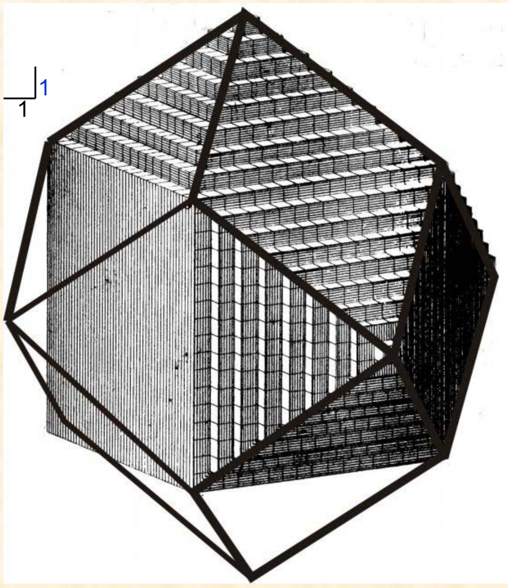


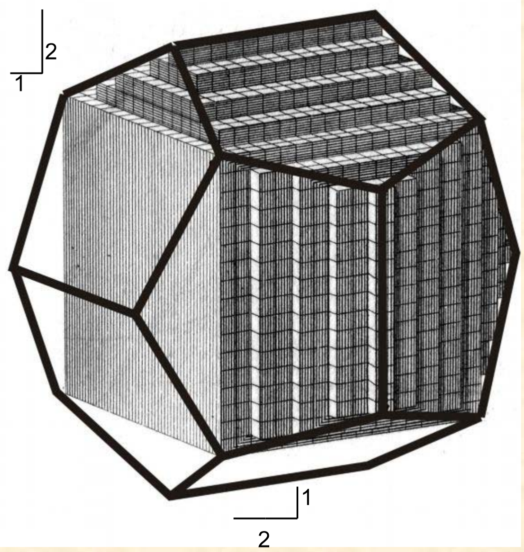


calcite scalenohedron
1784

The space–filling approach

Crystals are triperiodic assemblies of small blocks





Integrant molecules,
Law of decrements (Haüy 1784)

Polar theory – the 7 crystal systems

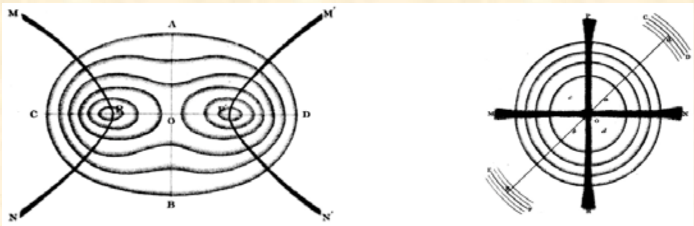
- No ultimate atom, dynamic equilibrium of matter resulting from the action of forces centred at poles, and oriented relative to the main cleage planes and growth faces – three main axes (four for the hexagonal system)

C. S. Weiss (1780-1856)
(1815)

F. Mohs (1773-1839)
(1821)

Optical systems = Crystal systems

D. Brewster
(1781-1868)



Biaxial crystals nitre (KNO3)	Uniaxial crystals calcite
Orthorhombic Monoclinic Triclinic	Hexagonal Tetragonal Trigonal

(1818)

Laws of polarization and double refraction

The Brewster angle

The 32 crystal classes

M. L. Frankenheim (1801-1869)

Order of the axes of rotation: 1, 2, 3, 4, 6

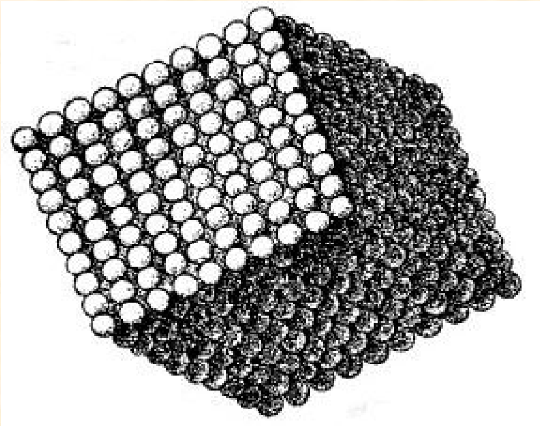
32 symmetries possible for a crystal:
Crystal *orders* = 32 crystal classes
(1826)

J. F. C. Hessel (1796-1872)

32 possible combinations of crystal axes of symmetry = 32 crystal classes
(1830)

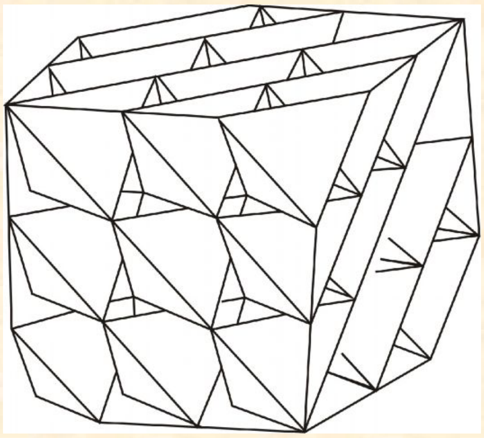
Notion of crystal lattice

L. A. Seeber (1793-1855)



Mathematical properties of lattices
(Positive ternary quadratic forms – 1824)

G. Delafosse (1796-1878)



Notion of merohedry (1843) –

structure of a crystal of boracite (1843)
$Mg_3B_7O_{13}Cl$ – space group *Pca*21 –
pyroelectric (and piezoelectric)

•The 14 lattice modes – 1848

A. Bravais (1811-1863)

- Regular systems of points
- Theory of crystal lattices
- Symmetry of crystal lattices
- Polar lattice

•The 14 lattice modes – 1848

A. Bravais (1811-1863)

• The 65 proper space groups – 1879

L. Sohncke (1842-1897)

Sohncke: The orientation of the distribution of points around a given point of a regular system of points may vary.

C. Jordan (1838-1922): Screw axes and the notion groups of motion (1867)

Sohncke: the 65 proper groups of motion (space groups)

•The 14 lattice modes – 1848

A. Bravais (1811-1863)

• The 65 proper groups of motion (space groups) – 1879

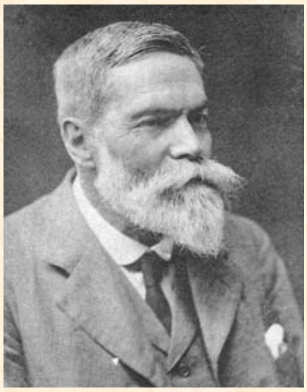
L. Sohncke (1842-1897)

• The 230 space groups

1891 1891 1894

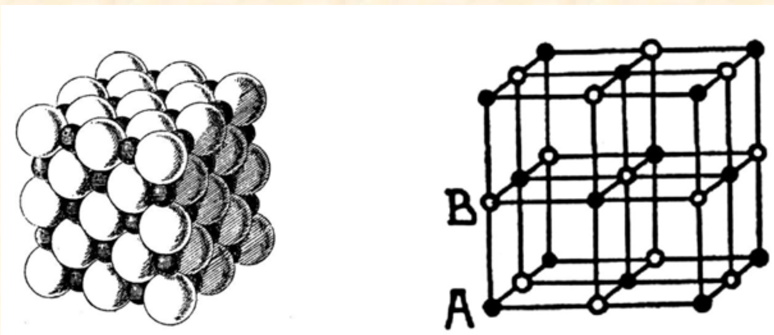
A. M. Schoenflies (1853-1928)

E. S. Fedorov (1853-1919)



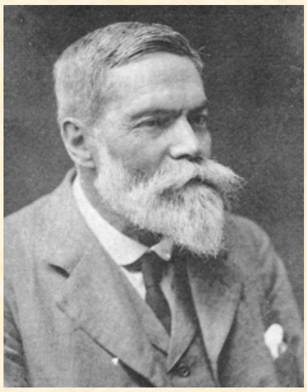
W. Barlow (1845-1934)

The close–packing approach



Structure of NaCl

W. Barlow (1897) W. L. Bragg (1913)



W. Barlow (1845-1934)

W. Barlow and the chemist W. H. Pope (1870-1939) discussed the correlation between chemical constitution and chemical form (1906-1910)

X-rays: Waves or corpuscles?

Discovery W. C. Röntgen 8 November 1895 – Würzburg University (Germany) kkn

Wilhelm C. Röntgen (1845-1923)
1901 Nobel Prize Physics

Mrs Röntgen's hand

Authier – XTOP 2014

X-rays: Waves or corpuscles?

Discovery W. C. Röntgen 8 November 1895 – Würzburg University (Germany)

Waves

Impulse theory: E. Wiechert (1896),
G. G. Stokes (1896),
J. J. Thomson (1898)

Theory of scattering:
J. J. Thomson (1898, 1903)

J. J. Thomson (1856-1940)
1906 Nobel Prize Physics

Electromagnetic waves produced by moving charges: A. Liénard (1898)

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X-ray polarization (1905),
characteristic X-ray lines (1909)
C. G. Barkla

Charles G. Barkla (1877-1944)
1917 Nobel Prize Physics

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Theory of diffraction (1900-1912)
A. Sommerfeld
from diffraction experiment:
$\lambda \sim 0.4$ Å

A. Sommerfeld (1868-1951)

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Corpuscles?

X-rays are neutral pairs (one α particle + one β particle): W. H. Bragg (1907)

William Henry Bragg (1862-1941)

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Corpuscles?

X-rays are neutral pairs (one α particle + one β particle): W. H. Bragg (1907)

X-rays are light quanta: W. Wien (1907)
J. Stark (1907)
$\lambda \sim$ 0.6 Å

X-rays are material bodies: J. Stark (1909)

Compton scattering: A. H. Compton (1923)

Dual nature of X-rays: L. de Broglie (1924)

Munich in 1912

Institute for Mineralogy

P. von Groth

1843-1927

Munich in 1912

Institute for Mineralogy (P. von Groth)

Institute of Experimental Physics (W. C. Röntgen)

P. Koch chief assistant (PhD 1901)
E. Wagner (PhD 1903)
W. Friedrich (PhD 1911)
P. Knipping (PhD1913)
R. Glocker (PhD 1914)

Munich in 1912

Institute for Mineralogy (P. von Groth)

Institute of Experimental Physics (W. C. Röntgen)

Institute of Theoretical Physics

P. Debye, first assistant, 1906 - 1911
M. Laue, *Privatdozent*, from 1909
W. Friedrich, assistant, from 1911
P. P. Ewald, student, from 1909

Arnold Sommerfeld

1868-1951

Munich in 1912

Friedrich

Ewald

Epstein

Sommerfeld

Ewald's thesis : *To find the optical properties of an anisotropic arrangement of isotropic resonators (Sommerfeld 1910)*

In other words, to relate a physical property (double refraction) to crystallographic properties: the periodic nature of crystals and the anisotropy of biaxial and uniaxial crystals.

Ewald's thesis : *To find the optical properties of an anisotropic arrangement of isotropic resonators (Sommerfeld 1910)*

Peter Paul Ewald (1888-1985)

Dispersion und Doppelbrechung von Elektronengittern (Kristallen).

Inaugural-Dissertation

zur

Erlangung der Doktorwürde

einer

hohen philosophischen Fakultät (II. Sektion)

der Königl. Ludwigs-Maximilians-Universität zu München

eingereicht am 16. Februar 1912

von

Peter Paul Ewald.

Göttingen 1912.

Druck der Dieterichschen Universitäts-Buchdruckerei

(W. Fr. Kaestner).

Authier – XTOP 2014

Ewald's thesis : *To find the optical properties of an anisotropic arrangement of isotropic resonators (Sommerfeld 1910)*

1) Theory of dispersion (propagation in an infinite medium)

2) Theory of refraction and reflection
(propagation in a semi-infinite medium – incident wave)

The progressive wave propagating inside the crystal is the sum of two terms:

a) a term propagating with velocity *c*, which cancels out the incident wave (extinction theorem)

b) a term propagating with phase velocity *c/n*

Ewald's Thesis

The term propagating with phase velocity *c/n*

Das Gesamtpotential (the optical field)

$$(7)\qquad \Pi = -\frac{\pi}{2abc}\sum_{l,\,m,\,n}^{-\infty\,..\,+\infty} \frac{e^{-i\frac{l\pi+a\alpha}{a}x - i\frac{m\pi+b\beta}{b}y - i\frac{n\pi+c\gamma}{c}z}}{k_0^2 - \left(\frac{l\pi+a\alpha}{a}\right)^2 - \left(\frac{m\pi+b\beta}{b}\right)^2 - \left(\frac{n\pi+c\gamma}{c}\right)^2}$$

(reproduced in *Ann. Phys.* (1916). **49***, page 22)*

$$\sum_{\mathbf{h}} \frac{[\exp -2\pi \mathrm{i}\, \mathbf{K_h}\cdot\mathbf{r}]}{K_h^2 - k^2}$$

Sum of plane waves of wave vectors $\mathbf{K_h}$ ($K_h \sim n\,k$).

It will be called wave-field by Laue later (1931)

• **Question of *Ewald* to *Laue*** (end of January 1912)

Is my treatment correct?

• **Question back of *Laue* to *Ewald***:

What is the distance between the resonators?

About 1/1000th of the wavelength of visible light (Ewald)

What would happen if you asumed very much shorter wavelengths to travel in the crystal? (Laue)

• **Ewald's answer: the theory would hold, look at equation (7)**

Laue's intuition

• The periodic distribution of the dipoles in a crystal is remindful of a grating.

• Interference occurs if the period of the grating and the wavelength are close.

My intuition for optics suddenly gave me the answer: lattice spectra would have to ensue…I immediately told Ewald that I anticipated the occurrence of interference phenomena with X-rays. (Laue, Nobel lecture)

Laue's assumption

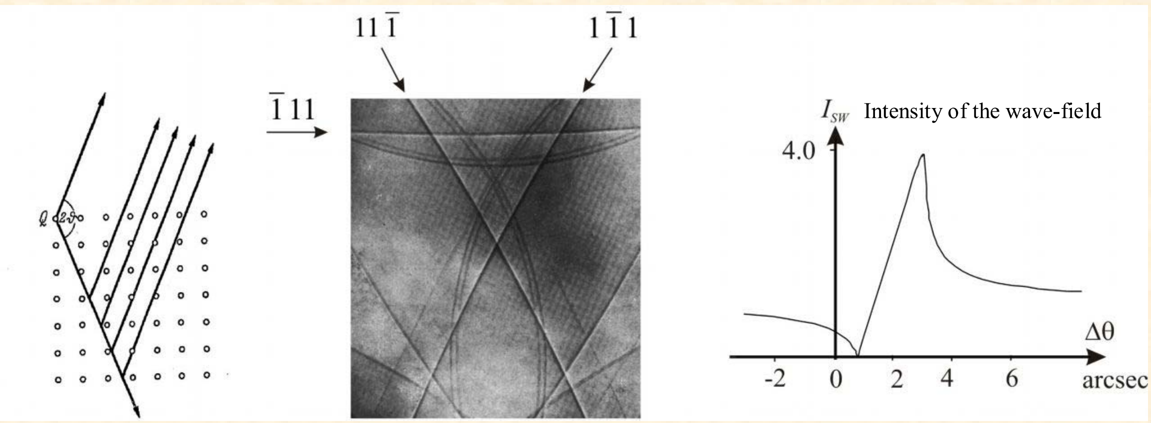
Since we thought it would have something to do with fluorescence radiation, we chose a crystal with a heavy metal in order to produce an intense homogeneous secondary radiation, ($CuSO_4$, 5 H_20)

(*W. Friedrich*, *P. Knipping*, *M. Laue* - 8 June 1912)

Laue thought that the interferences would be due to characteristic lines which would excite fluorescence. In fact, as shown by W. L. Bragg (November 1912), they were due to white light, the *Bremsstrahlung* background of the X-ray beam.

Laue's assumption

Laue's initial idea was therefore that there would be interference between the waves emitted by lattice sources. This is the origin of the Kossel lines, first observed by G. Borrmann for X-rays (1935) and interpreted by Laue using the properties of wave-fields (1935).



Lattice sources | Kossel lines | Origin of the black-white contrast

W. Friedrich — 1883 – 1968

Sommerfeld's assistant
PhD with Röntgen

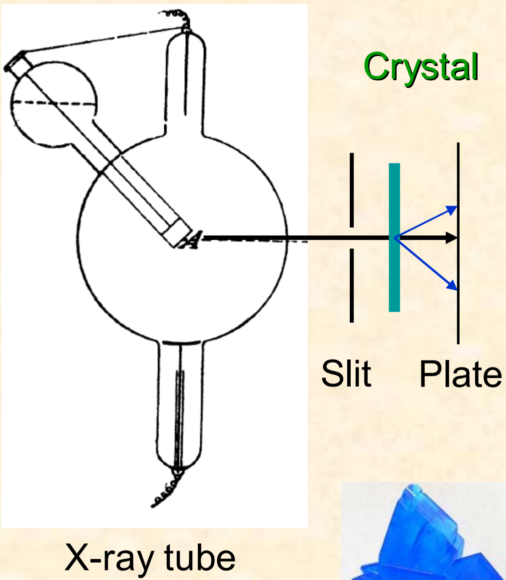
P. Knipping — 1883 – 1935

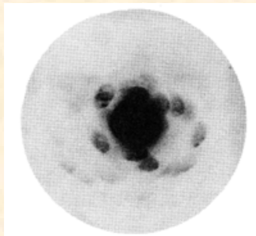
Student with Röntgen
PhD with Röntgen

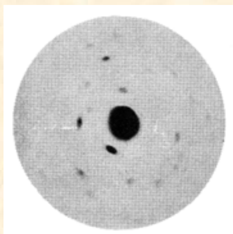
M. Laue — 1879 - 1960

Privatdozent in
Sommerfeld's Institute
PhD with Planck

W. Friedrich, P. Knipping, M. Laue

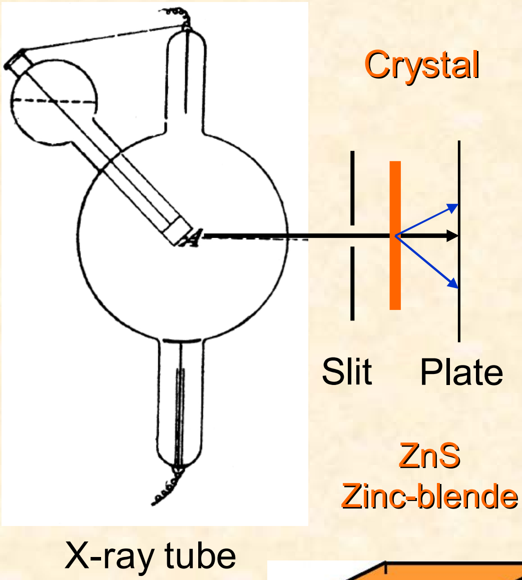


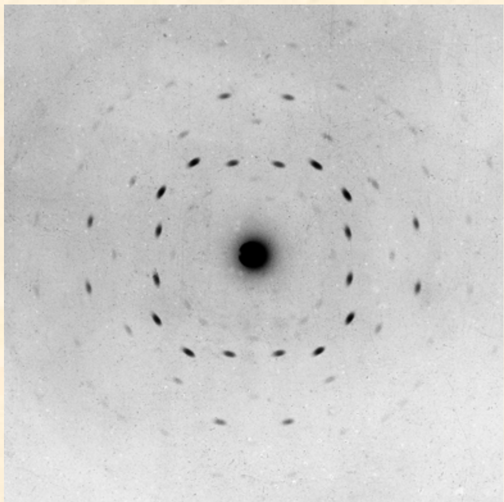


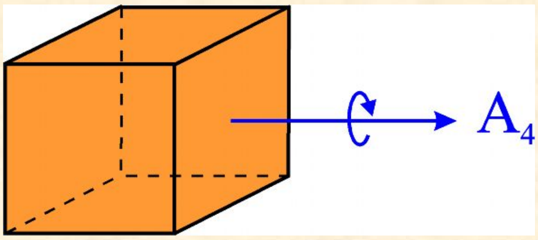


$CuSO_4$, 5 H_20

W. Friedrich, P. Knipping, M. Laue







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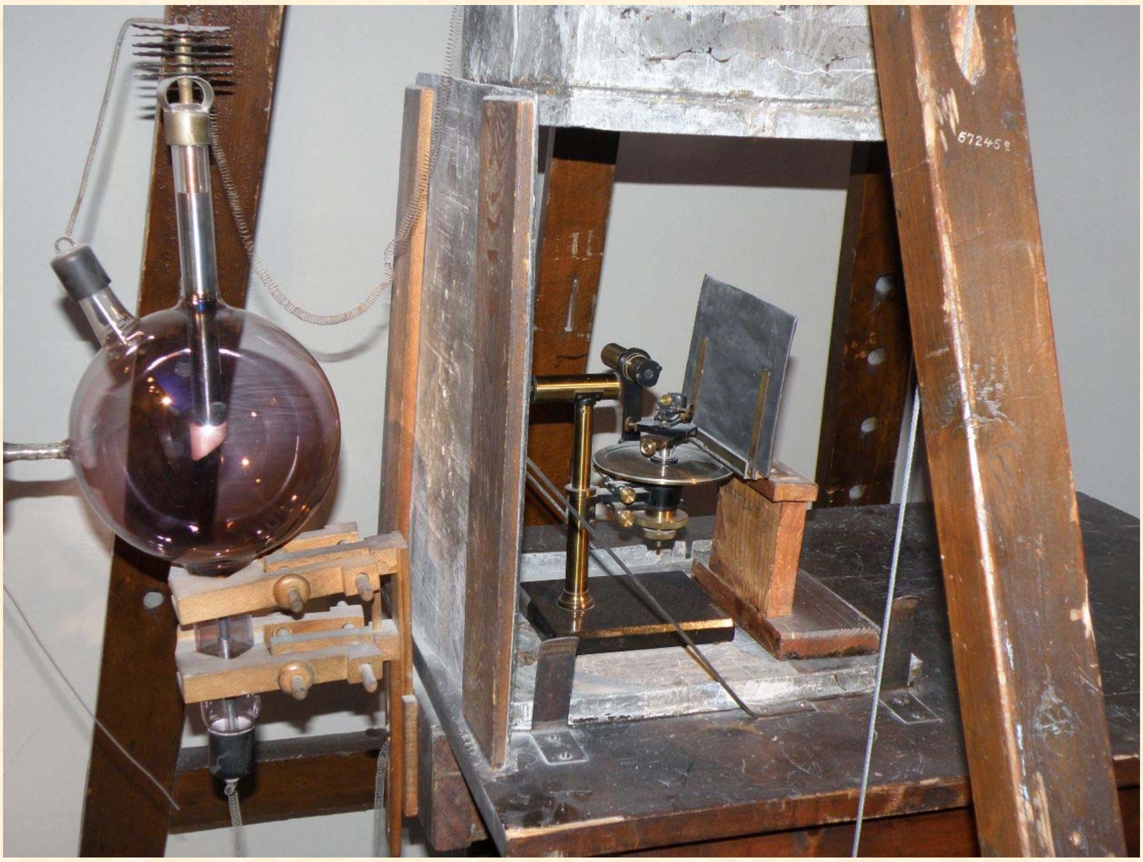
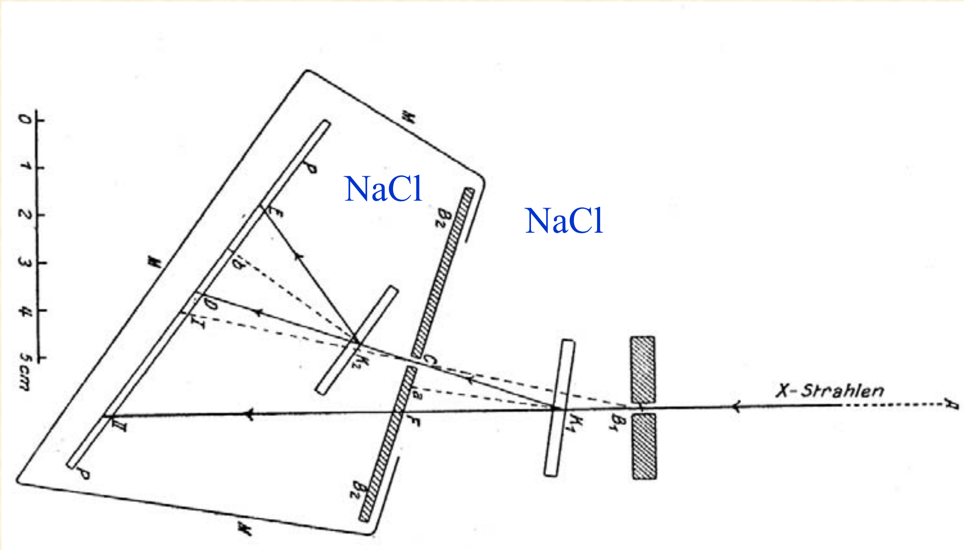


Reactions

May 1912 *Groth* was elated. *Röntgen* : *But those are not interference phenomena. They look different to me.* Röntgen was finally convinced by the work of the Braggs and by E. Wagner and R. Glocker's double crystal experiment in his own Institute in 1913.



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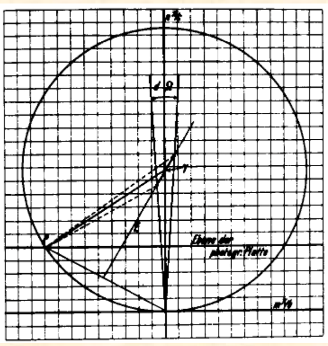
8 June 1912 First publication: experiment + intensity (geometrical theory)

14 June 1912 *Laue* gives a talk to the *Physikalische Gesellschaft* in Berlin. *Planck*: *Everyone of us felt that a remarkable feat had been achieved*

Mid June 1912 *Sommerfeld* gives a talk in Göttingen; *Ewald* introduces the **Ewald sphere** and the **reciprocal lattice** (published in 1913)

$$\sum_{\mathbf{h}} \frac{[\exp -2\pi i\, \mathbf{K_h}\cdot\mathbf{r}]}{K_h^2 - k^2}$$



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21 June 1912 *Einstein*: *The photograph is so sharp that one would have scarcely have suspected it, due to thermal agitation*

26 June 1912 *Laue* gives a talk in Würzburg; *L. Vegard* informs *W.H. Bragg* of the discovery

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May 1912 *Groth* was elated. *Röntgen* : *But those are not interference phenomena. They look different to me.* Röntgen was finally convinced by the work of the Braggs and by E. Wagner and R. Glocker's double crystal experiment in his own Institute in 1913.

8 June 1912 First publication: experiment + intensity (geometrical theory)

14 June 1912 *Laue* gives a talk to the *Physikalische Gesellschaft* in Berlin. *Planck*: *Everyone of us felt that a remarkable feat had been achieved*

Mid June 1912 *Sommerfeld* gives a talk in Göttingen; *Ewald* introduces the **Ewald sphere** and the **reciprocal lattice** (published in 1913)

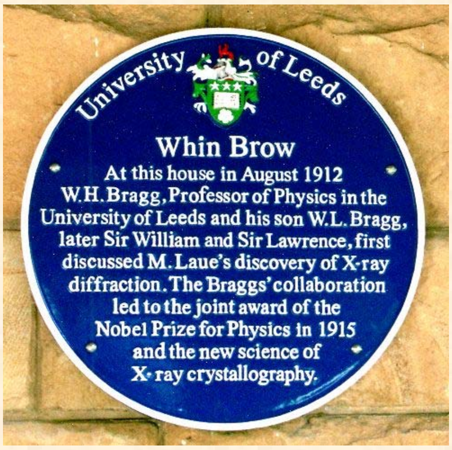
21 June 1912 *Einstein*: *The photograph is so sharp that one would have scarcely have suspected it, due to thermal agitation*

26 June 1912 *Laue* gives a talk in Würzburg; *L. Vegard* informs *W.H. Bragg* of the discovery

6 July 1912 Second publication: the three Laue equations

Reactions

August 1912 *W. H. and W. L. Bragg*, father and son, discuss Laue's experiment



The house where the Braggs spent the summer 1912 on the Yorkshire coast

Reactions

August 1912 *W. H. and W. L. Bragg*, father and son, discuss Laue's experiment

26 August 1912 *J. Stark* writes up his interpretation of the Laue diagrams as due to corpuscular rays

October 1912 Exchange of letters between *W. H. Bragg* and *Laue*:
W. H. Bragg to Laue: *the interference diagram is due to Bremsstrahlung and does not depend on the nature of the anticathode material* (quoted by Laue, 15 October 1912)

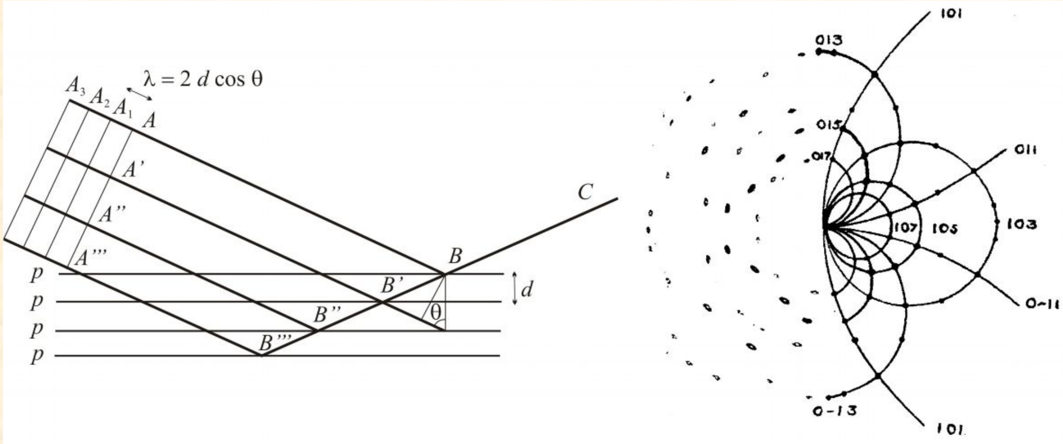
24 October 1912 Letter of *W. H. Bragg* to *Nature*: *the directions of the secondary pencils are avenues between the crystal atoms.*

11 November 1912 *J. J. Thomson* communicates *W. L Bragg*'s paper deriving Bragg's law to the Cambridge Philosophical Society

11 November 1912 ***W. L Bragg*'s paper deriving Bragg's law**

The crystal selects the appropriate wavelengths from the white spectrum: *The explanation which I propose, on the contrary, assumes the existence of a continuous spectrum over a wide range in the incident radiation; the crystal acts as a diffraction grating*.

Diffraction of pulses: *When a pulse falls on a number of particles scattered over a plane, the secondary waves from them will build up a wave front, exactly as if part of the pulse had been reflected from the plane, as in Huygens' construction for a reflected wave.*



Reactions

24 November 1912 Letter of *G. Wulff* to *Z. Kristallogr*. showing that Laue's indices h_1, h_2, h_3 define a crystallographic orientation

28 November 1912 Letter of *W. H. Bragg* to *Nature* suggesting dual nature, wave and corpuscular, of X-rays

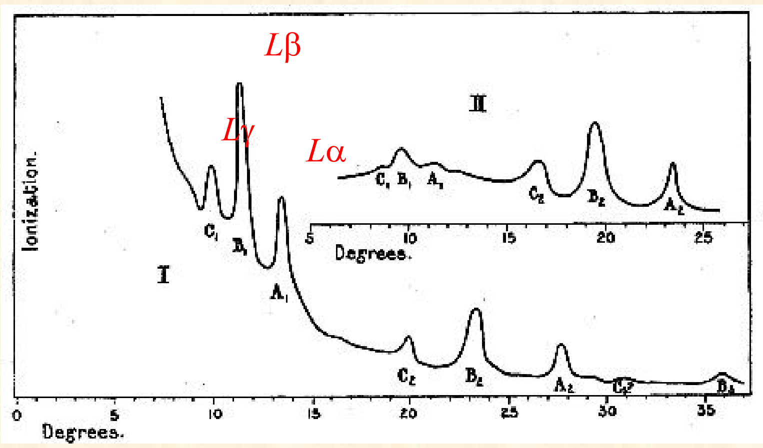
W. H. Bragg 1921 *On Mondays, Wednesdays, and Fridays we use the wave theory; on Tuesdays, Thursdays, and Saturdays we think in streams of flying energy quanta or corpuscles.* (Robert Boyle Lecture)

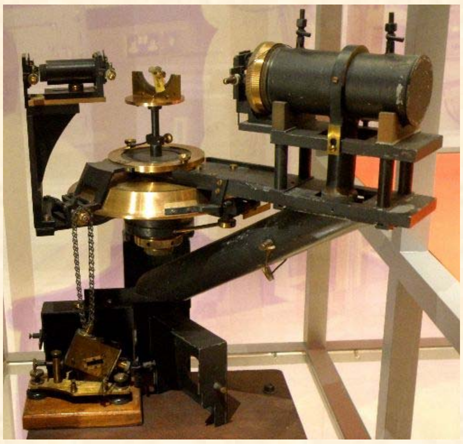
1 March 1913 *Laue*, in an addendum to the reprint of the 1912 article: *The lattice elements (Gitterelemente) have chosen a finite number of wavelengths out of the infinite number of wavelengths in the incident beam.*

1 April 1913 *Laue* derives Bragg's law and shows its equivalence with his 3 equations

Selective reflection of characteristic lines

17 April 1913 first X-ray spectrum *W. H.* and *W. L. Bragg*





Reflection of platinum radiation by NaCl- I: 100; II: 111

W. H. and *W. L. Bragg* → Structure determinations

X-ray Spectroscopy

01 July 1913 Spectrum of platinum *H. G. J. Moseley* and *C. G. Darwin*

H. G. J. Moseley (1887-1915) - in Manchester (1913-1914)

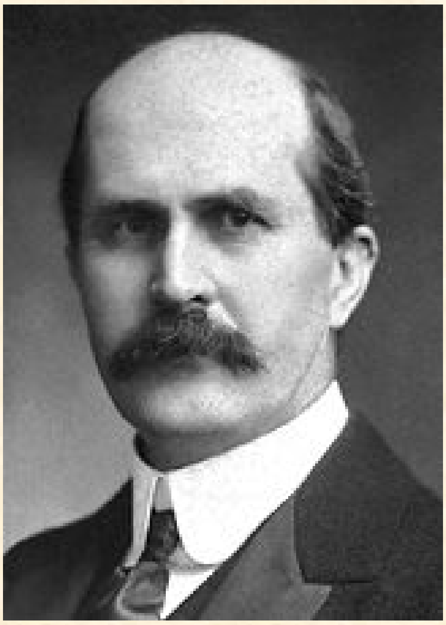
High frequency spectra of the elements

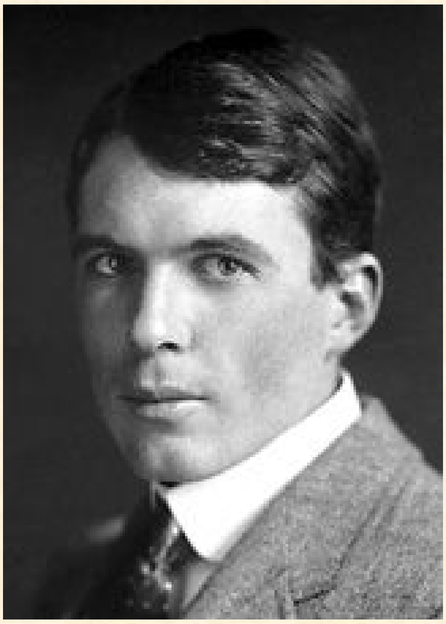
Moseley's law

Attribution of atomic numbers

Missing elements

The first structure determinations



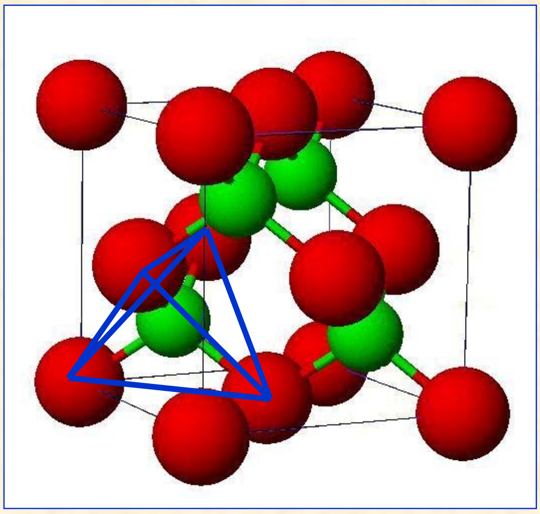


William Henry Bragg (1862-1941)   William Lawrence Bragg (1890-1971)

Nobel Prize Physics 1915

The first structure determinations

June 1913 *W. L. Bragg* (in Cambridge)

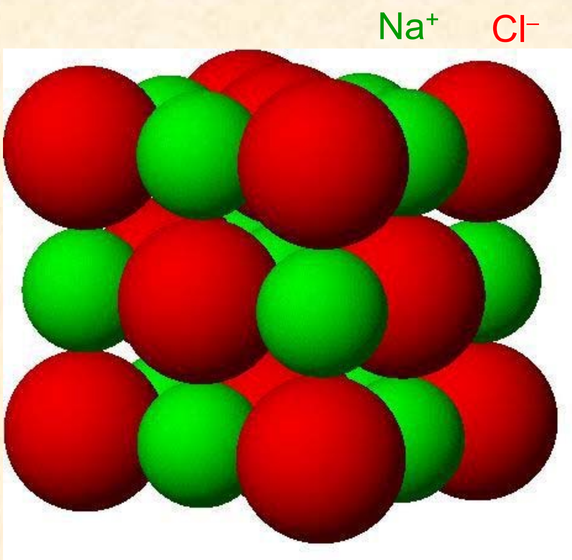


Zinc-blende, ZnS

The first structure determinations

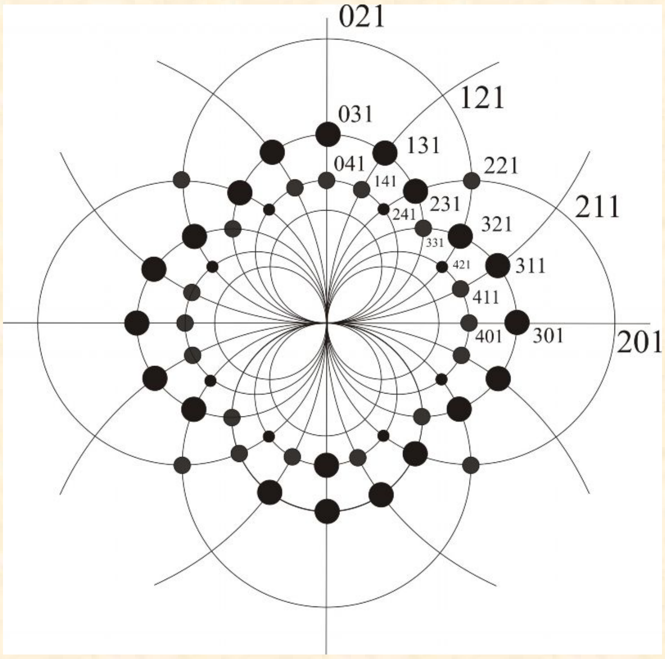
June 1913 *W. L. Bragg*

Halite (NaCl)

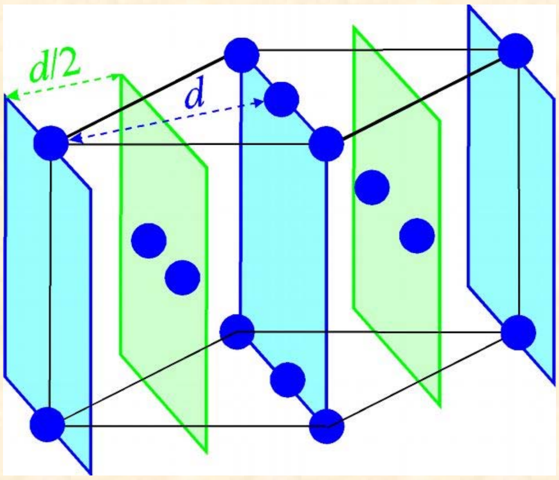


NaCl, KCl, KBr

How were determined the first structures?



Laue pattern of KCl (Bragg 1913)

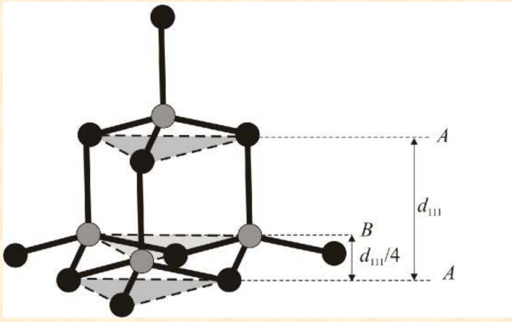


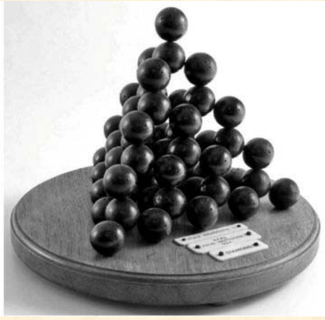
Face-centered cubic crystal

$Z(Na^+) = 10$, $Z(Cl^-) = 18$;
$Z(K^+) = 18$, $Z(Cl^-) = 18$;

The first structure determinations

September 1913 *W. H. Bragg* (in Leeds) and *W. L. Bragg* (in Cambridge)

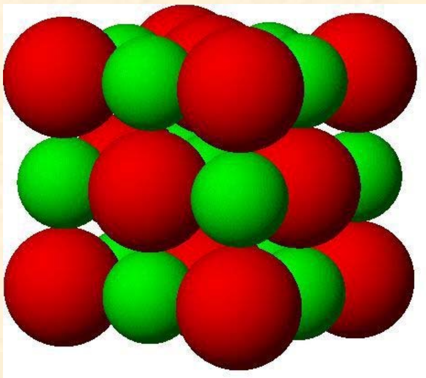




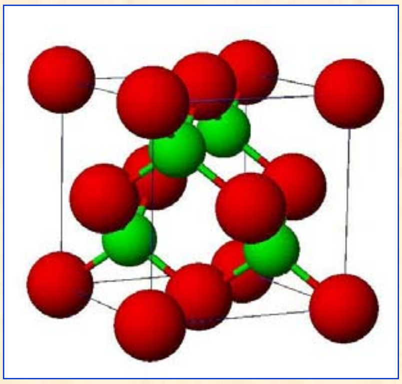
Diamond

Tetravalency of carbon

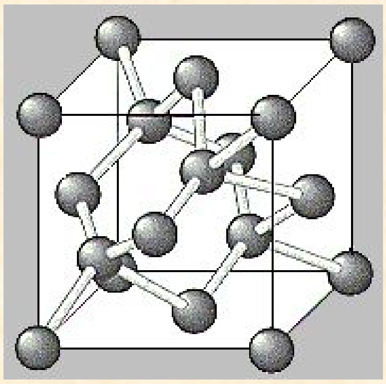
The first structures



NaCl



ZnS



Diamond

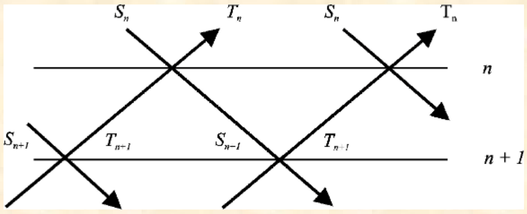
No individual molecules

H. E. Armstrong (1927): *more than repugnant to the common sense, not chemical cricket*

Darwin – 1914

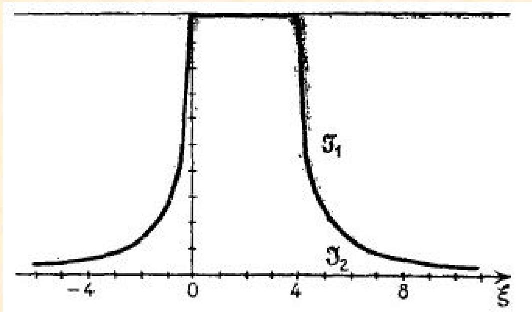
1) Geometrical theory
2) Diffraction by a perfect crystal (dynamical theory)

C. G. Darwin (1887-1962)



Recurrence equations

Total reflection



(Ewald 1917)

Ewald – dynamical theory of X-ray diffraction

Sir G. G. Stokes (1849): 'On the dynamical theory of diffraction'.

J. C. Maxwell (1865): 'A dynamical theory of the electromagnetic field'.
It is a dynamical theory, because it assumes that in that space there is matter in motion, by which the observed electromagnetic phenomena are produced .

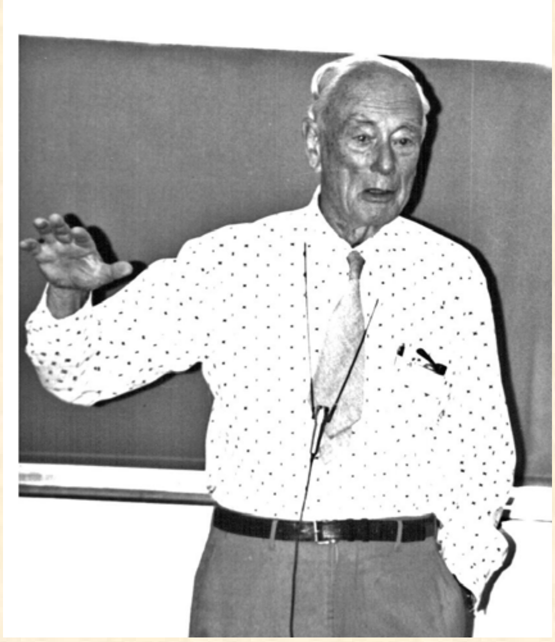
P. P. Ewald (1975): *Dynamical theory is part of General Optics.*

Ewald – dynamical theory of X-ray diffraction

1914 – *Sommerfeld's X-ray installation was taken to an improvised hospital. I went along and learned to do medical work*.

1915 – *I was ordered to Russia as field X-ray mechanic. As my X-ray wagon did not appear, I had plenty of time and enjoyed Königsberg and the good marzipan and worked out the theory of reflection and refraction on a half crystal.*

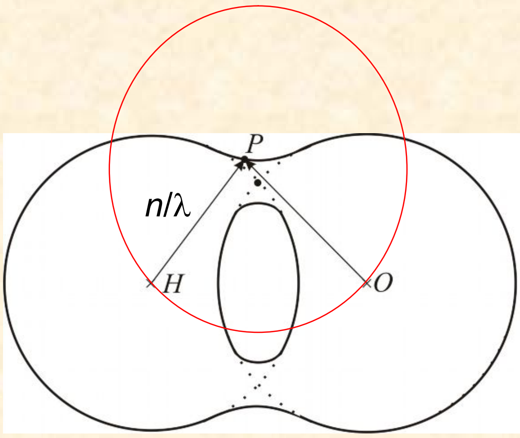
1916 – *On the Russian front, I had a quiet time, and I could go on with the theory of dispersion and that is where it originated.*



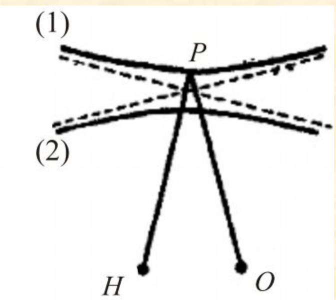
P. P. Ewald at the 1975 Limoges summer school (ancestor of XTOPs)

Ewald – dynamical theory of X-ray diffraction

Ewald sphere

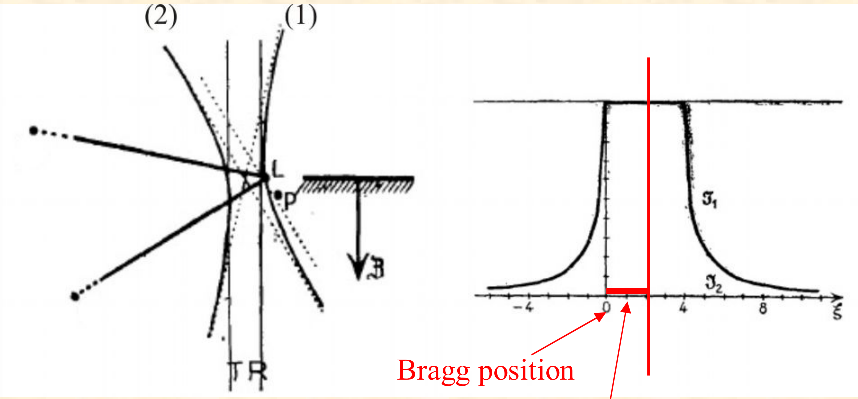


Dispersion surface



Ewald – dynamical theory of X-ray diffraction

Reflection geometry



1) Total reflection

2) Deviation from Bragg's angle $\delta\theta$

Refraction of X-rays

Index of refraction : $n = 1 - \delta$; $\delta = R\lambda^2 F_o / 2\pi V = 2\,\delta\theta \approx 10^{-5}$

Deviation from Bragg's angle

First observed *W. Stenström* (1919); *E. Hjalmar* (1920) – *M. Siegbahn*

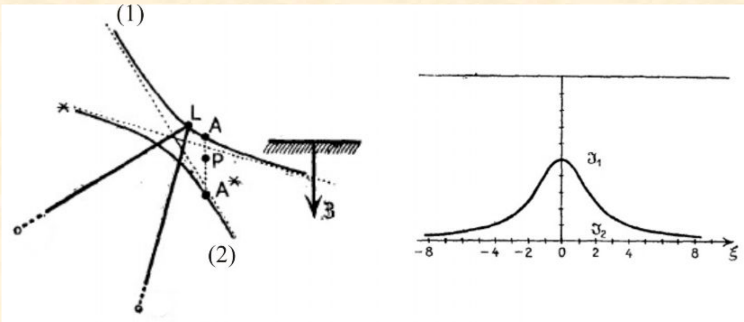
calculated *Ewald* (1920)

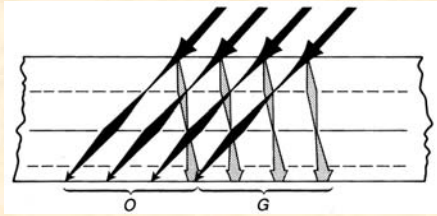
Direct measurement with a glass prism *A. Larsson, M. Siegbahn* and *I. Waller* (1924)

Specular reflection glass, silver *A. H. Compton* (1922)

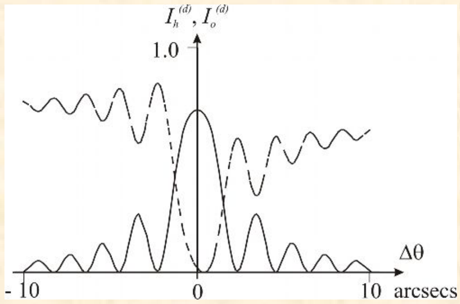
Ewald – dynamical theory of X-ray diffraction

Transmission geometry





Pendellösung *Ewald* 1917

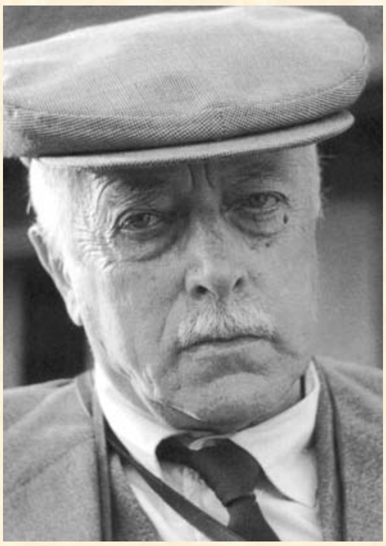


M. Lefeld-Sosnowska and *C. Malgrange* 1968

Laue – dynamical theory of X-ray diffraction - 1931

Properties of wave-fields

$$|D(r)|^2 = |D_o \exp(-2\pi \mathbf{K_o.r}) + D_h \exp(-2\pi \mathbf{K_h.r})|^2$$



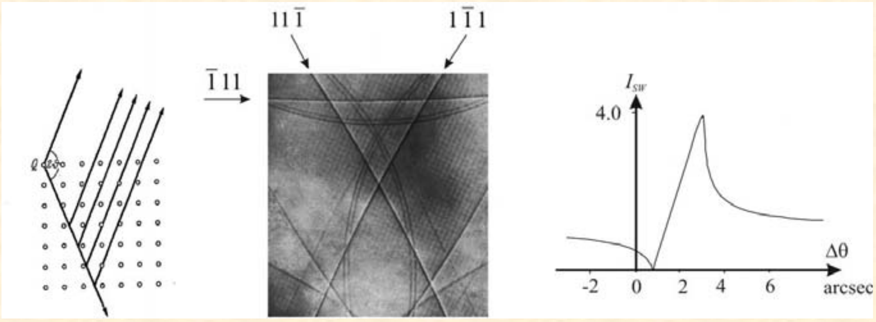
Laue – dynamical theory of X-ray diffraction - 1931

Properties of wave-fields

$$|D(r)|^2 = |D_o \exp(-2\pi\ \mathbf{K_o}.\mathbf{r}) + D_h \exp(-2\pi\ \mathbf{K_h}.\mathbf{r})|^2$$

Kossel lines

Lattice sources



Experiment: electrons *Kossel* and *Voges* 1935.

X-rays *Borrmann* 1935

Theory: *Laue* 1935

Laue – dynamical theory of X-ray diffraction - 1931

Properties of wave-fields

$$|D(r)|^2 = |D_o \exp(-2\pi\ \mathbf{K_o}.\mathbf{r}) + D_h \exp(-2\pi\ \mathbf{K_h}.\mathbf{r})|^2$$

Standing waves

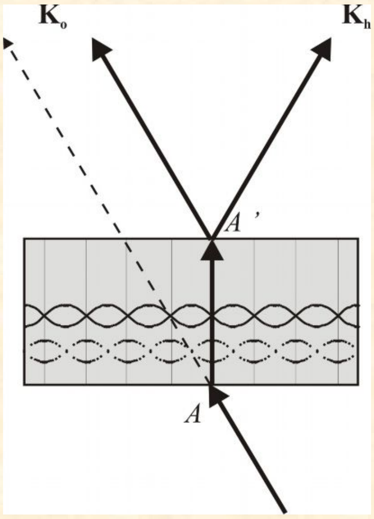
$$|D(r)|^2 = |D_o|^2 + |D_o|^2 + |D_o D_h|\ \cos (2\pi\ \mathbf{h}.\mathbf{r} + \psi)$$

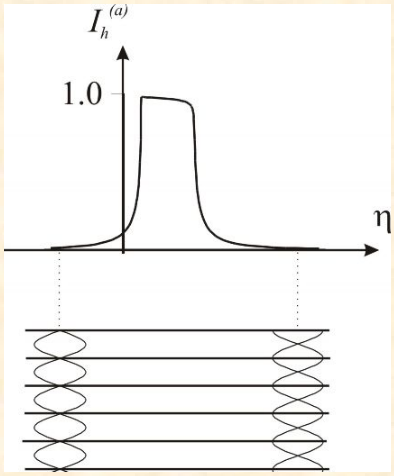
Laue – dynamical theory of X-ray diffraction - 1931

Standing waves $|D(r)|^2 = |D_o|^2 + |D_o|^2 + |D_oD_h| \cos(2\pi\, \mathbf{h.r} + \psi)$

Anomalous absorption *Borrmann* 1941

Branch 1
Branch 2



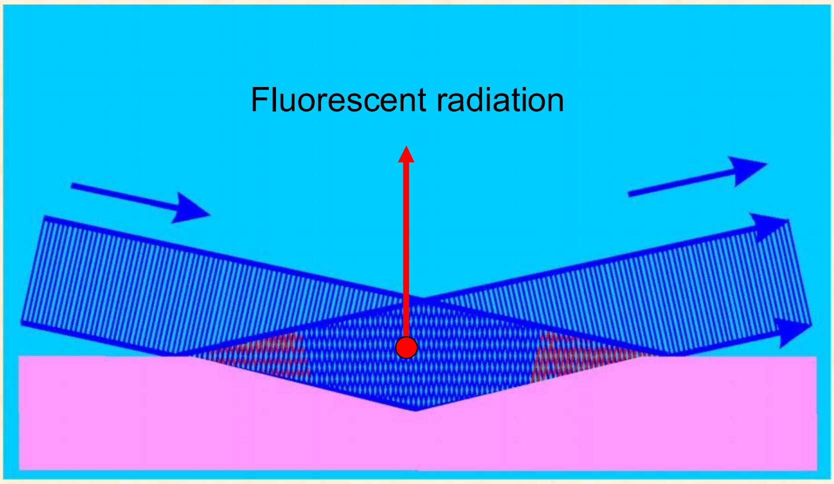


Branch 1 Branch 2

Laue – dynamical theory of X-ray diffraction - 1931

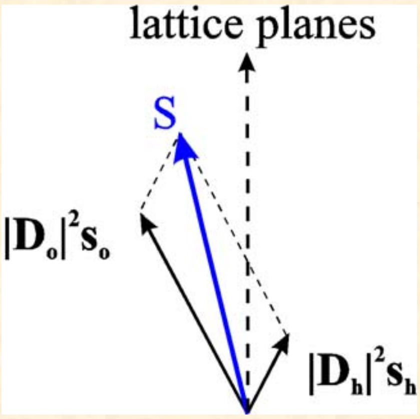
Standing waves $|D(r)|^2 = |D_o|^2 + |D_o|^2 + |D_oD_h| \cos(2\pi\, \mathbf{h.r} + \psi)$

Application to the location of atoms at surfaces and interfaces
B.W. Batterman 1969



Laue – dynamical theory of X-ray diffraction - 1931

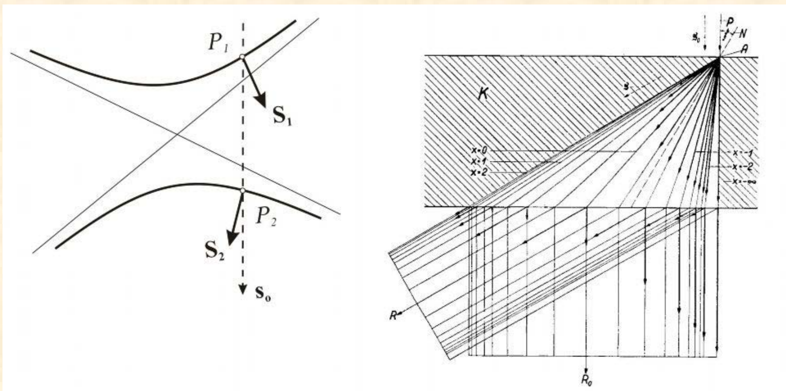
Propagation of wave-fields
Poynting vector *Laue* 1952



Laue – dynamical theory of X-ray diffraction - 1931

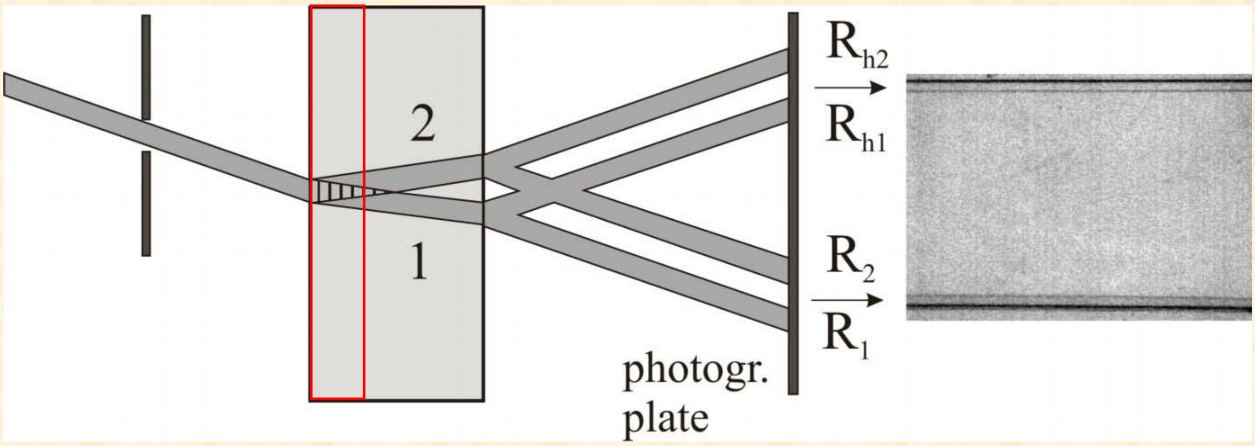
Propagation of wave-fields
Borrmann fan 1959

Gerard Borrmann
(1908-2006)

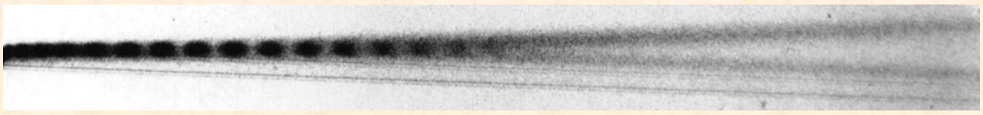


Laue – dynamical theory of X-ray diffraction - 1931

Double refraction of X-rays Prediction *Borrmann* 1955
Observation *Authier* 1960

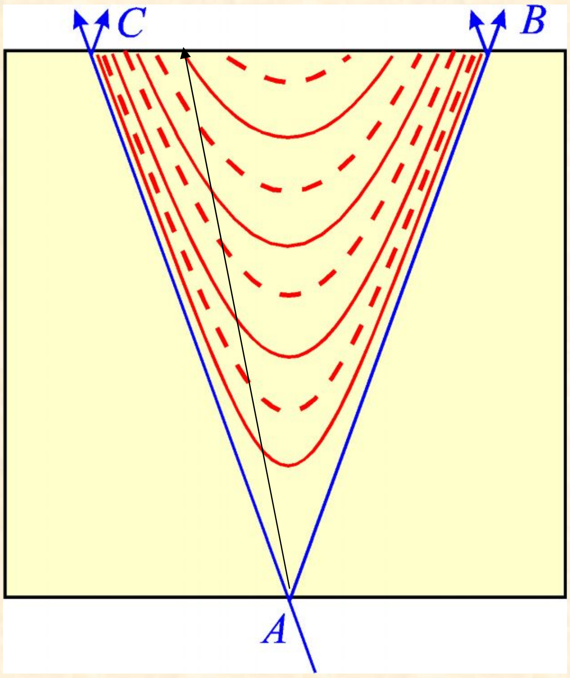


Plane wave Pendellösung *Malgrange* and *Authier* 1965

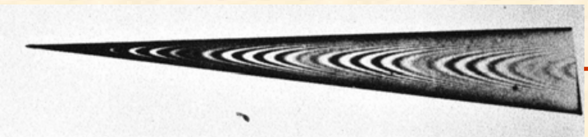


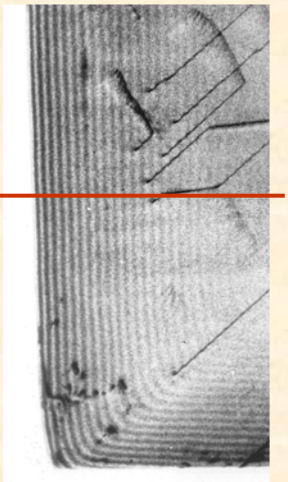
Kato – spherical waves - 1960

Norio Kato
(1923-2002)



Kato – spherical waves - 1960





Spherical waves Pendellösung *Kato* and *Lang* 1959