X-ray Diffraction and Crystal Structures

Week of October 18, 2010

Atomic and Nuclear Physics Laboratory (Physics 4780)

The University of Toledo
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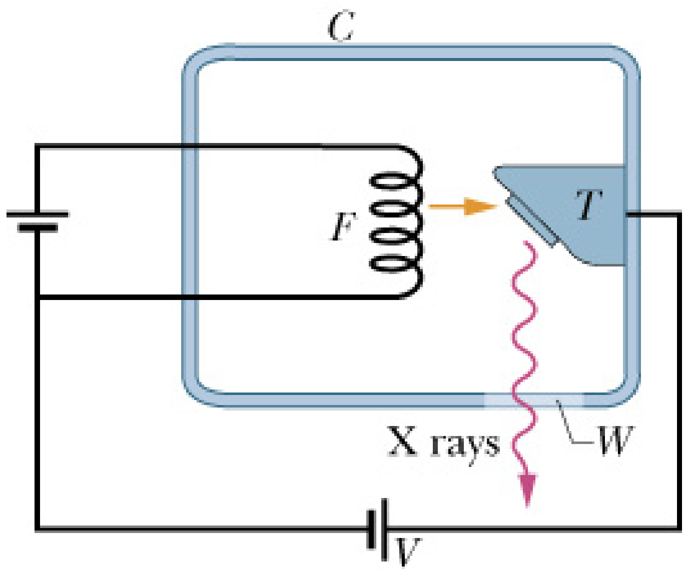
X-Ray Generation

X-rays are electromagnetic radiation with wavelength ~1 Å = 10^{-10} m
(visible light ~5.5×10^{-7} m)

X-ray generation



X-ray wavelengths too short to be resolved by a standard optical grating

$$\theta = \sin^{-1}\frac{m\lambda}{d} = \sin^{-1}\frac{(1)(0.1\text{ nm})}{3000\text{ nm}} = 0.0019°$$

X-Ray Generation

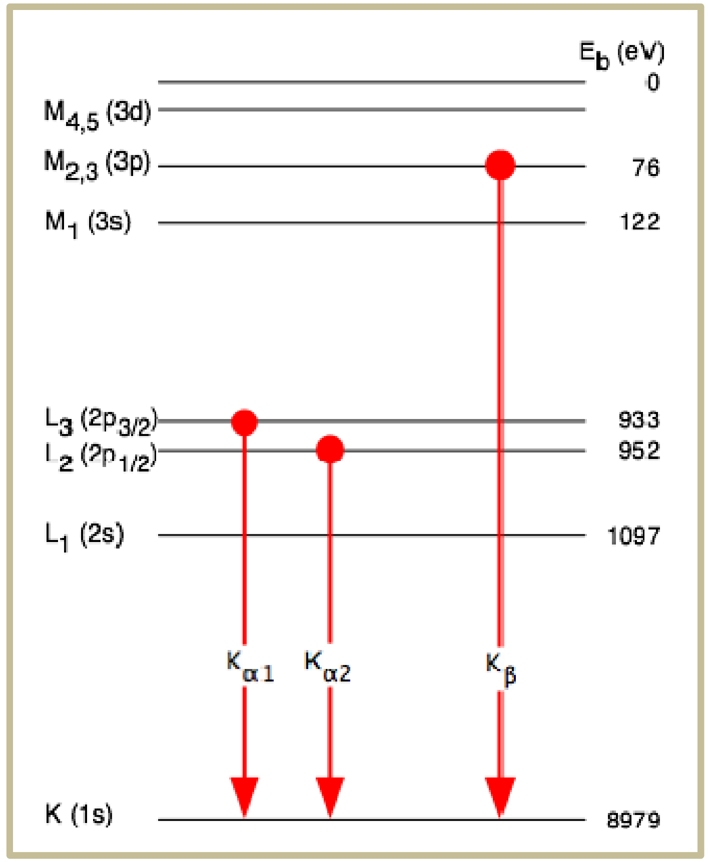
The most common metal used is copper, which can be kept cool easily, due to its high thermal conductivity, and which produces strong K_α and K_β lines. The K_β line is sometimes suppressed with a thin (~10 μm) nickel foil.

- **K-alpha (K_α)** emission lines result when an electron transitions to the innermost "K" shell (principal quantum number 1) from a 2p orbital of the second or "L" shell (with principal quantum number 2).

- The K_α line is actually a doublet, with slightly different energies depending on spin-orbit interaction energy between the electron spin and the orbital momentum of the 2p orbital.

$$\lambda(K_\alpha) = 0.154 \text{ nm}$$

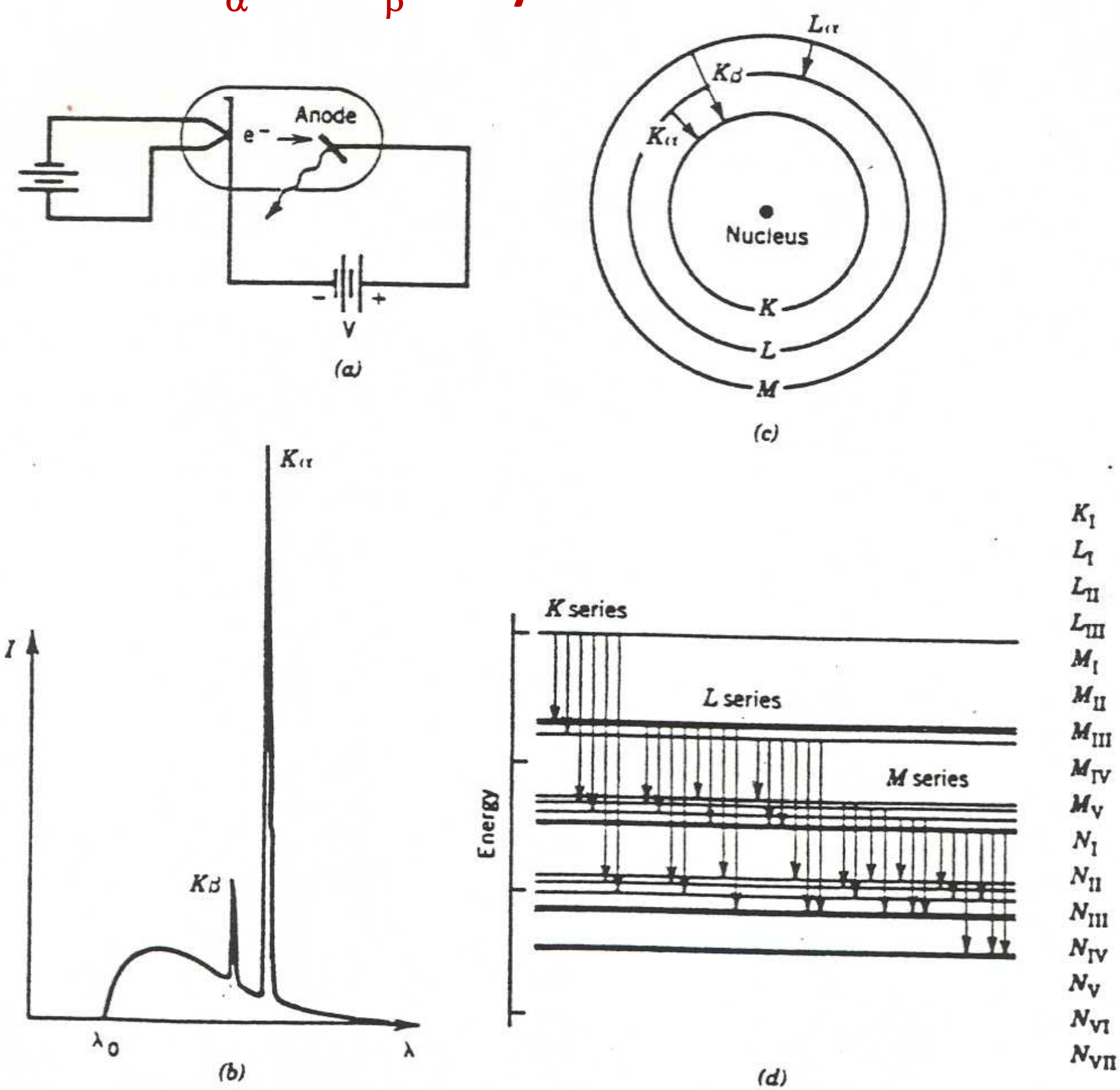
$$\lambda(K_\beta) = 0.139 \text{ nm}$$



Atomic levels involved in copper K_α and K_β emission.

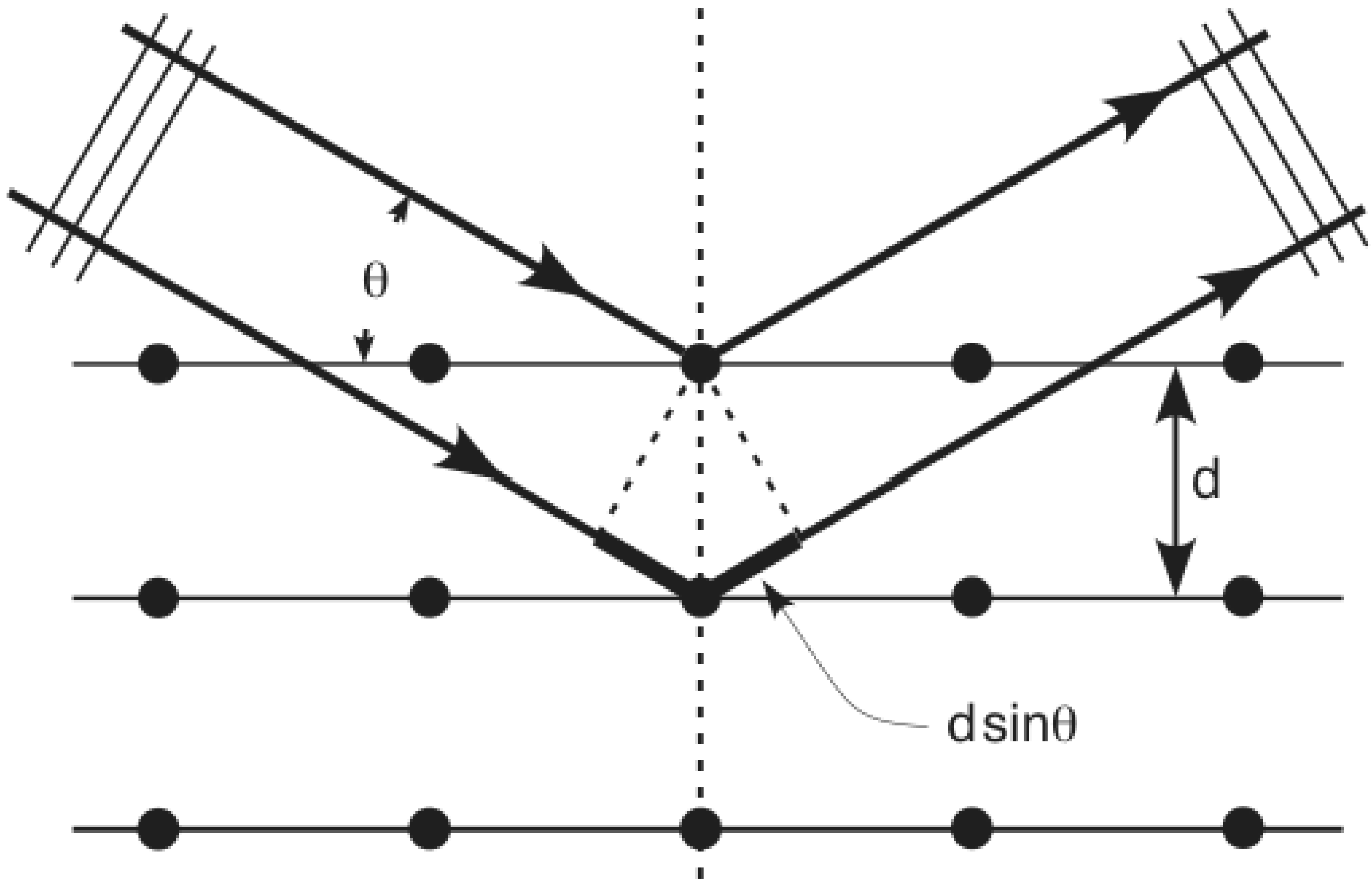
from http://en.wikipedia.org/wiki/K-alpha

K_α and K_β X-ray lines

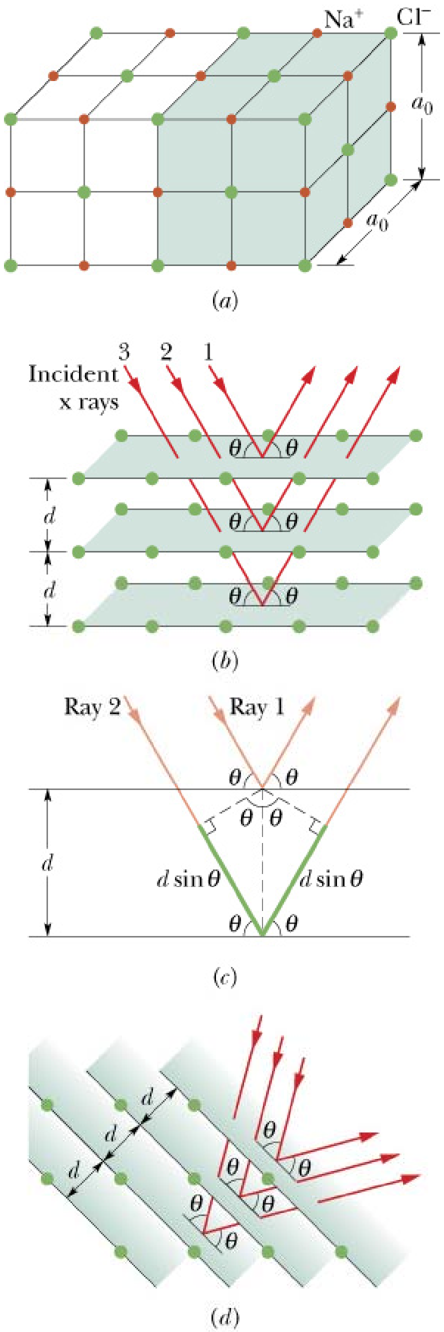


from Preston and Dietz, p. 191.

X-Ray diffraction



X-Ray Diffraction -- Bragg's Law



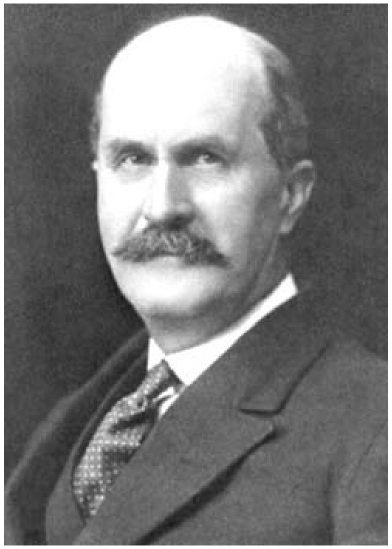
Diffraction of x-rays by crystal: spacing *d* of adjacent crystal planes on the order of 0.1 nm

⟶ three-dimensional diffraction grating with diffraction maxima along angles where reflections from different planes interfere constructively

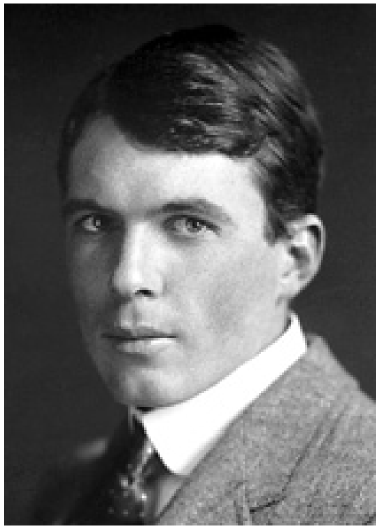
$2d \sin\theta = m\lambda$ for $m = 0, 1, 2, \ldots$

Bragg's Law

The Braggs (Bragg's Law)



Sir William Henry Bragg
1862 - 1942



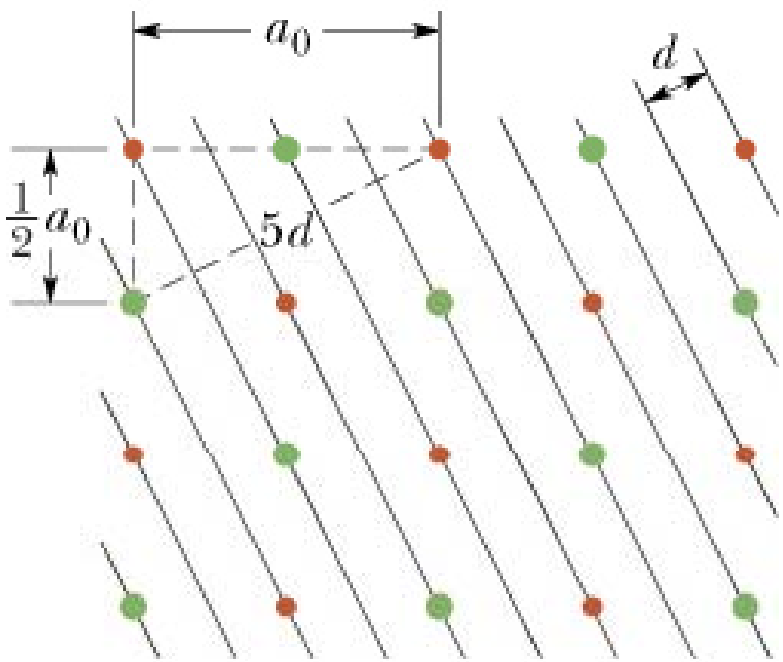
William Lawrence Bragg
1890 - 1971

Bragg occupied the Cavendish chair of physics at the University of Leeds from 1909. He continued his work on X-rays with much success. He invented the X-ray spectrometer and with his son, William Lawrence Bragg, then a research student at Cambridge, founded the new science of X-ray analysis of crystal structure.

In 1915 father and son were jointly awarded the Nobel Prize in Physics for their studies, using the X-ray spectrometer, of X-ray spectra, X-ray diffraction, and of crystal structure.

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

X-Ray Diffraction, cont'd



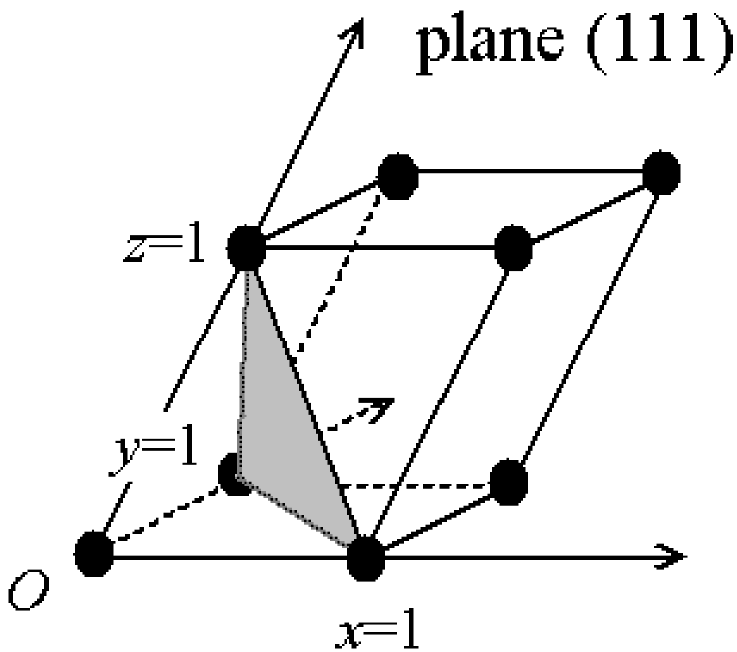
Interplanar spacing *d* is related to the unit cell dimensaion a_0

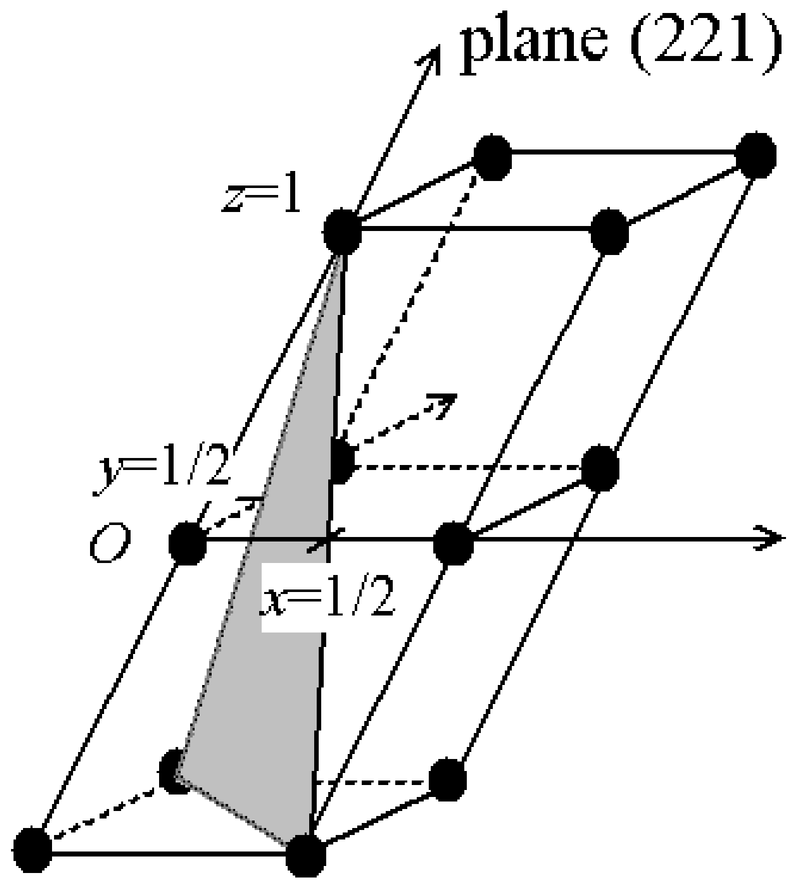
$$5d = \sqrt{\tfrac{5}{4}a_0^2} \quad \text{or} \quad d = \frac{a_0}{20} = 0.2236a_0$$

Not only can crystals be used to separate different x-ray wavelengths, but x-rays in turn can be used to study crystals, for example determine the type of crystal ordering and $a_{0.}$

Crystal structure, lattice planes, and Miller indices

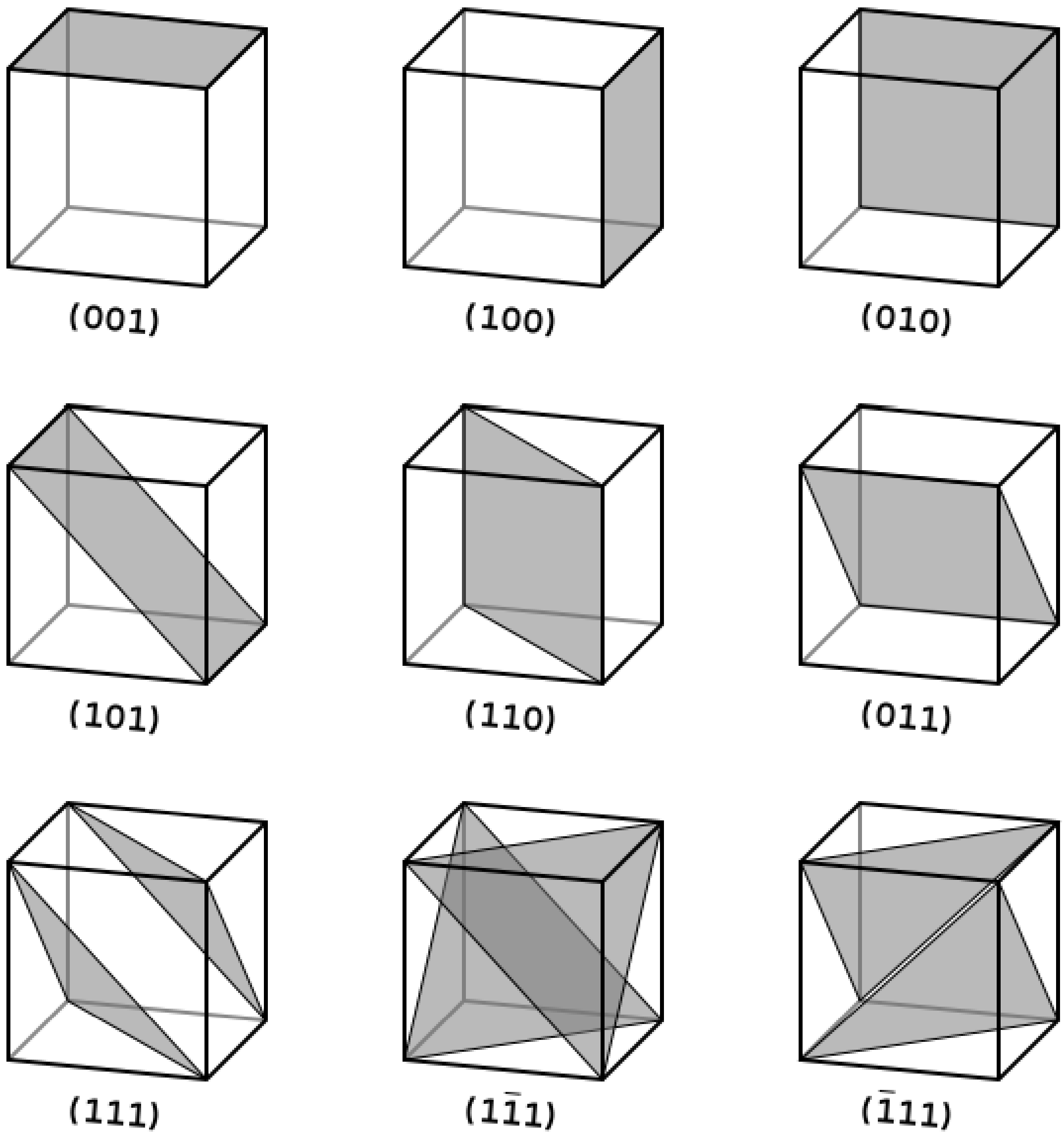
Planes with different Miller indices in cubic crystals. The *inverse* of these fractional intercepts yields the Miller indices *h, k, l*.





from http://en.wikipedia.org/wiki/Miller_index

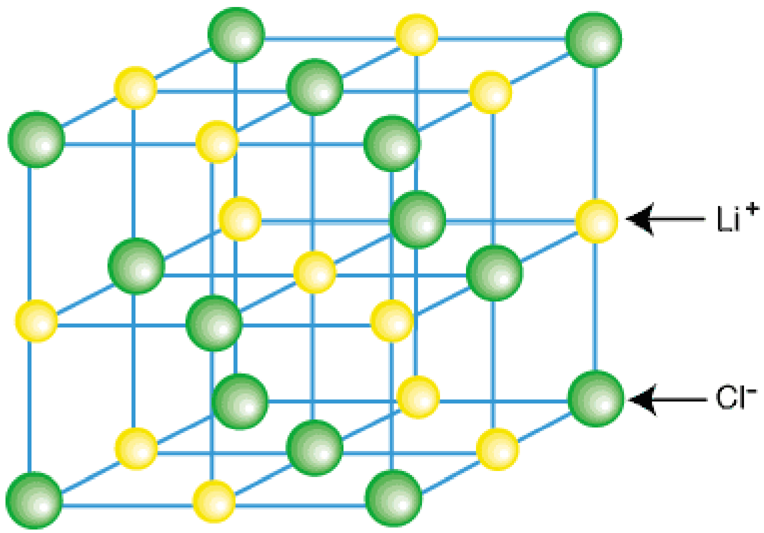
Crystal structure and Miller indices



Planes with different Miller indices in cubic crystals.

from http://en.wikipedia.org/wiki/Miller_index

Crystal structure and Miller indices



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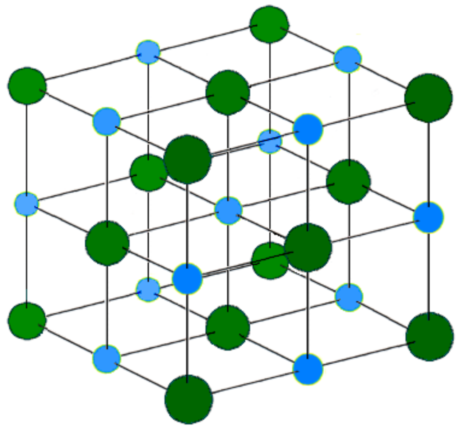
Indexing lattice planes

http://www.msm.cam.ac.uk/doitpoms/tlplib/miller_indices/lattice_index.php

Rock salt (cubic) crystal structure



$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

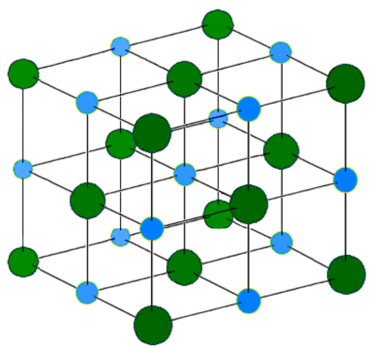
Structure factor for NaCl:

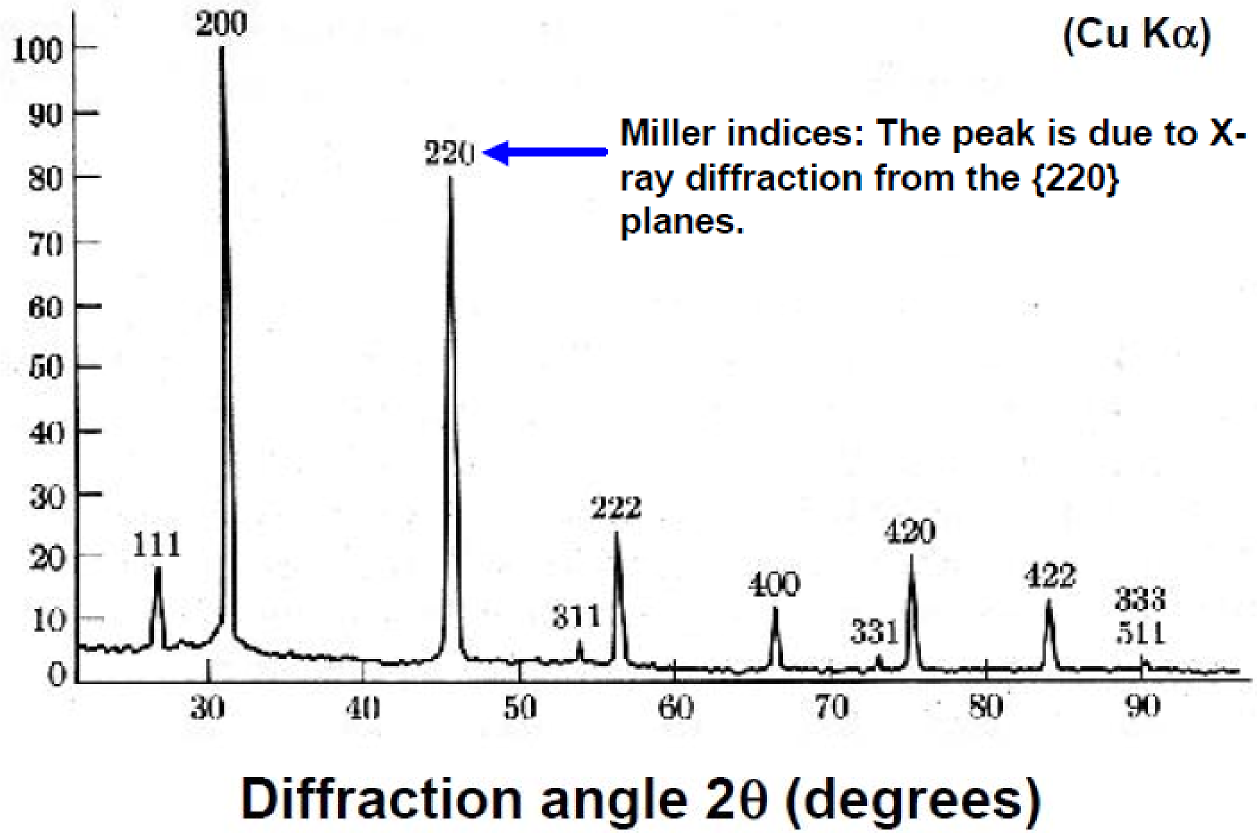
$$F = \left[f_{Na} + f_{Cl} e^{i\pi(h+k+l)} \right] \left[1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)} \right]$$

$$F = 4\left(f_{Na} + f_{Cl} \right) \quad \text{if } h, k, l \text{ are even}$$
$$F = 4\left(f_{Na} - f_{Cl} \right) \quad \text{if } h, k, l \text{ are odd}$$
$$F = 0 \quad \text{if } h, k, l \text{ are mixed}$$

X-Ray diffraction: a practical approach, by C. Suryanarayana, M. Grant Norton

X-Ray diffraction (XRD) pattern (diffractogram) from NaCl

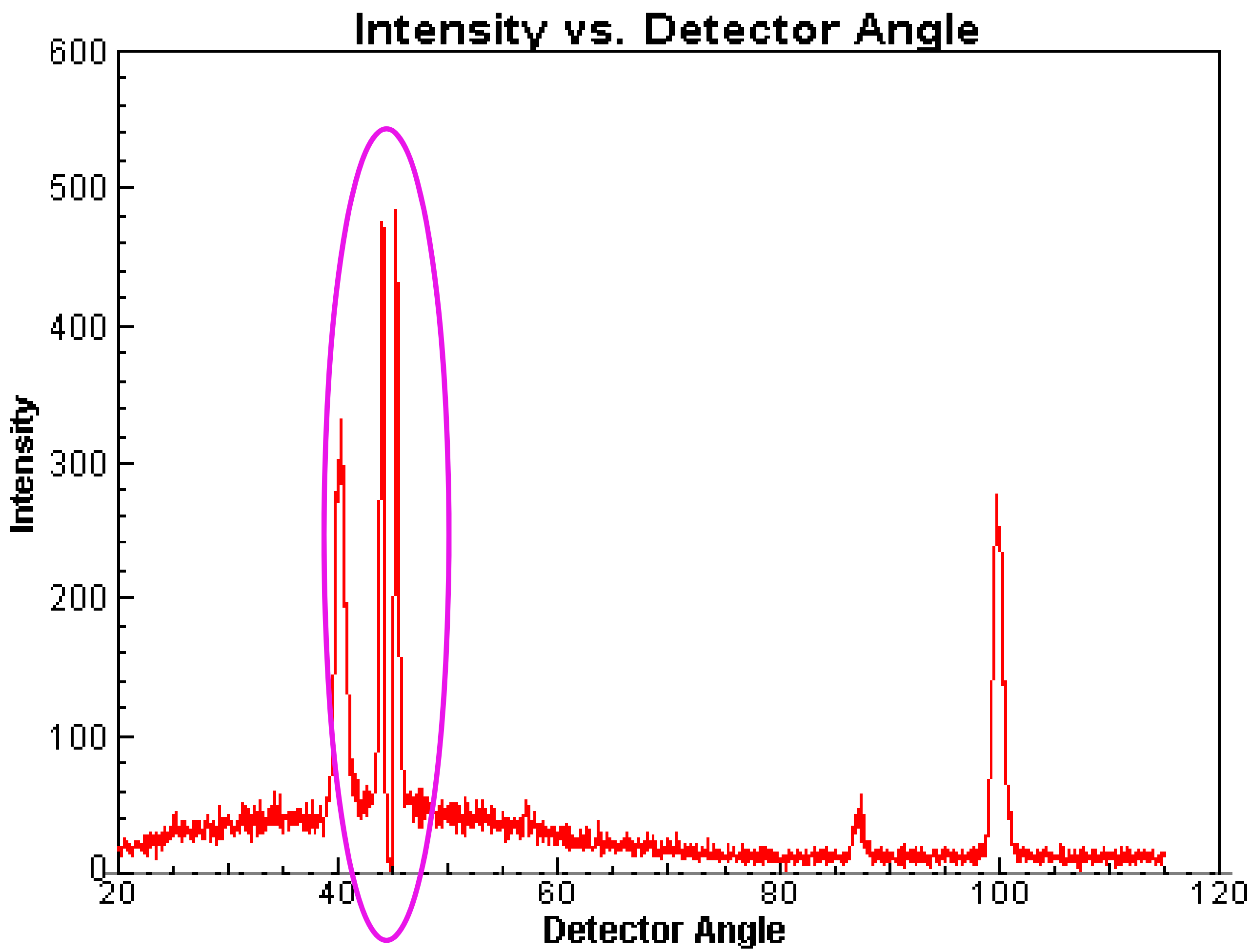




$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

http://web.pdx.edu/~pmoeck/phy381/Topic5a-XRD.pdf

LiF diffractogram (Cu K_α)



http://www.warren-wilson.edu/~physics/physics2/Formal2000/sstephens/lif.gif

TEL-X-Ometer

$K_{\alpha 1}$	1.540 Å
$K_{\alpha 2}$	1.544 Å
K_{β}	1.392 Å