Crystallographic Diffraction

Laue diffraction from a three-dimensional *abc* lattice grating

$$a\left(\cos\nu_1 - \cos\mu_1\right) = \mathbf{a}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = h\lambda$$
$$b\left(\cos\nu_2 - \cos\mu_2\right) = \mathbf{b}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = k\lambda$$
$$c\left(\cos\nu_3 - \cos\mu_3\right) = \mathbf{c}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = l\lambda$$

Max Laue, Walther Friedrich, and Paul Knipping (1912).

Bragg reflection from families of parallel *hkl* lattice planes

$$2d_{hkl}\sin\theta = n\lambda\,, \qquad 2\left(\frac{d_{hkl}}{n}\right)\sin\theta = \lambda\,, \qquad 2d_{nh\,nk\,nl}\sin\theta = \lambda$$

William Henry and William Lawrence Bragg (1913). (Father and son)

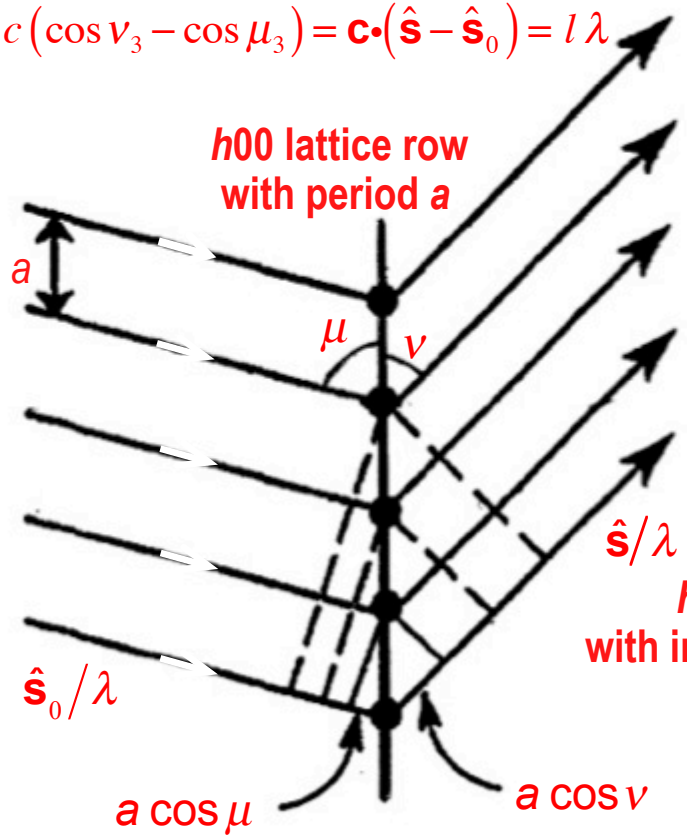
Integrated Bragg reflection intensities

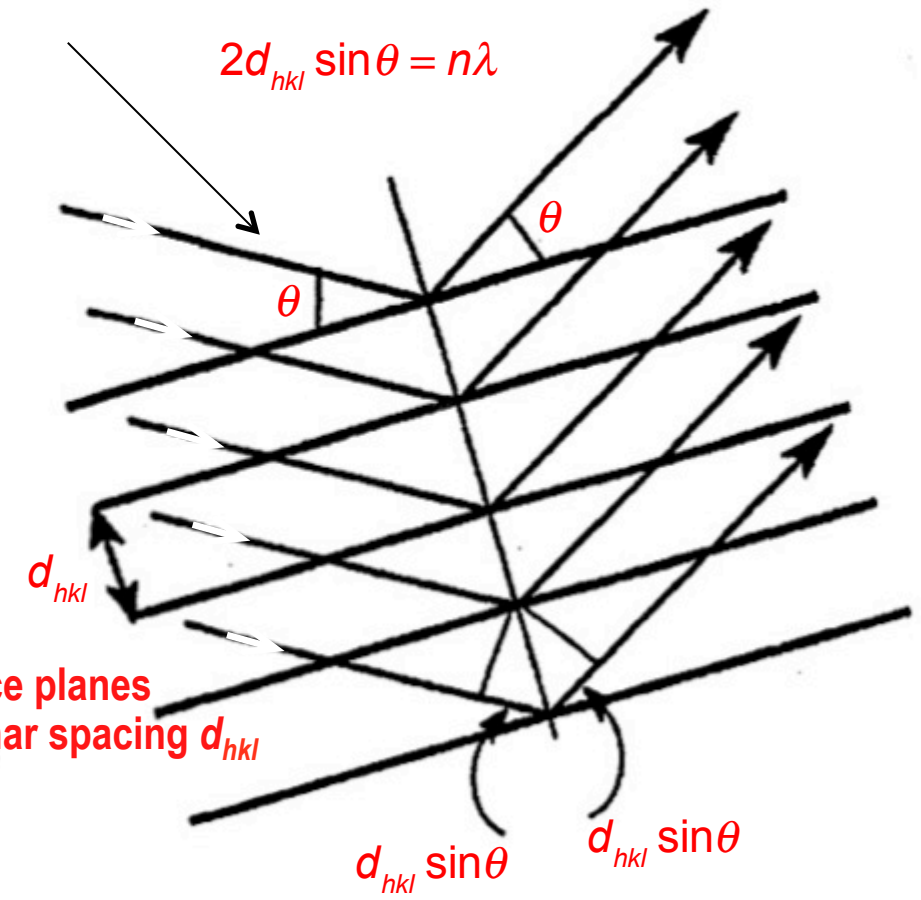
$$\rho = \frac{E\omega}{I_0} = kALp\left|F_{hkl}\right|^2 = \left(\frac{e^2}{mc^2}\right)^2 \lambda^3 \left(\frac{v_{\text{xtal}}}{V_{\text{cell}}}\right)^2 \left[\int_{v_{\text{xtal}}} \mathrm{e}^{-\mu(t_0+t_1)}\,\mathrm{d}v\right] \frac{1}{\sin 2\theta}\left(\frac{1}{2}+\frac{1}{2}\cos^2 2\theta\right)\left|F_{hkl}\right|^2$$

Charles G. Darwin (1914). (Grandson of the author of the theory of evolution)

Crystallographic diffraction

$$a\left(\cos\nu_1 - \cos\mu_1\right) = \mathbf{a}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = h\lambda$$
$$b\left(\cos\nu_2 - \cos\mu_2\right) = \mathbf{b}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = k\lambda$$
$$c\left(\cos\nu_3 - \cos\mu_3\right) = \mathbf{c}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = l\lambda$$



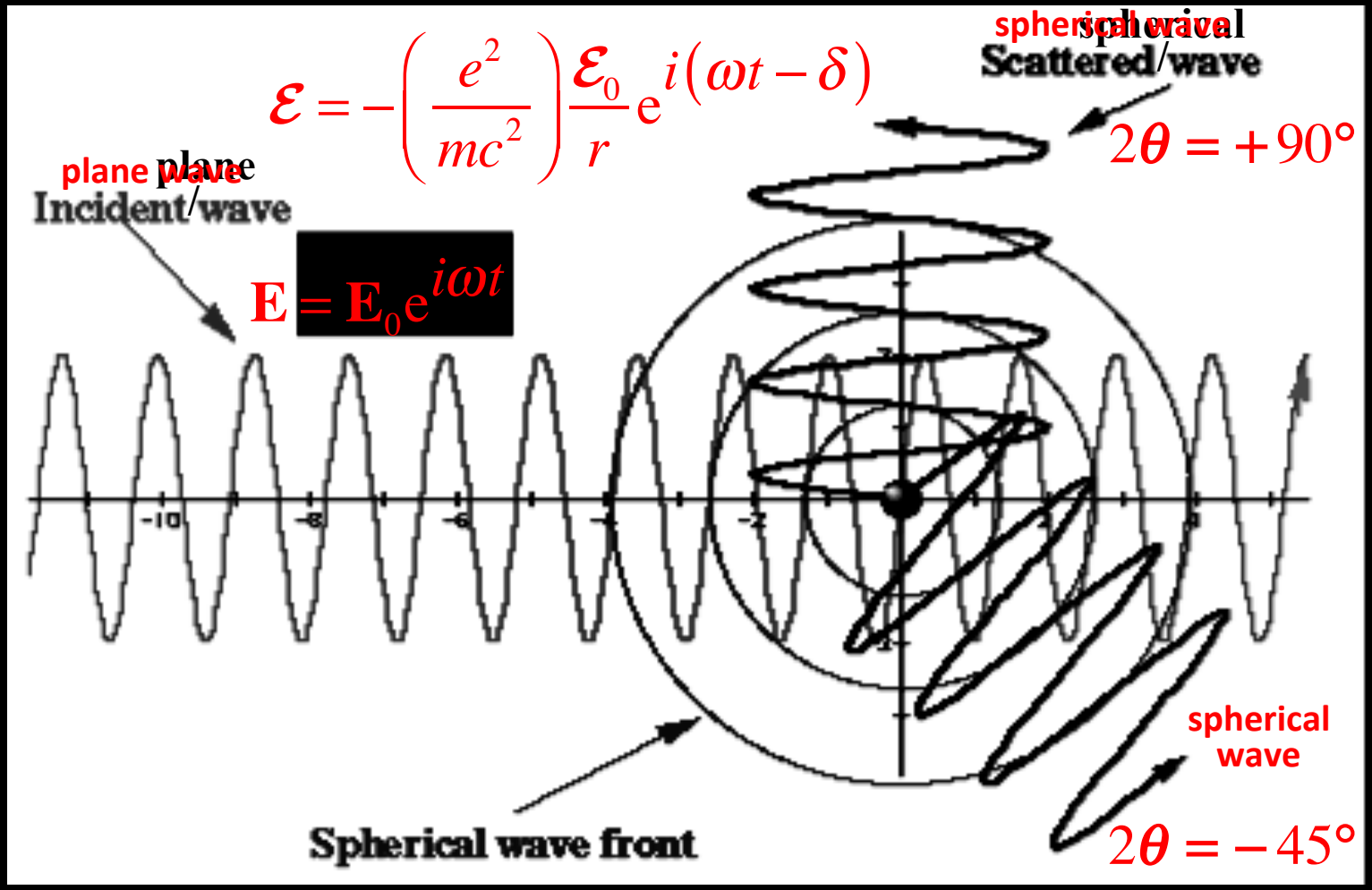


Laue transmission

Bragg reflection

Clegg, Blake, Gould & Main (2001). *Crystal Structure Analysis: Principles and Practice*, IUCr/Oxford Univ. Press.

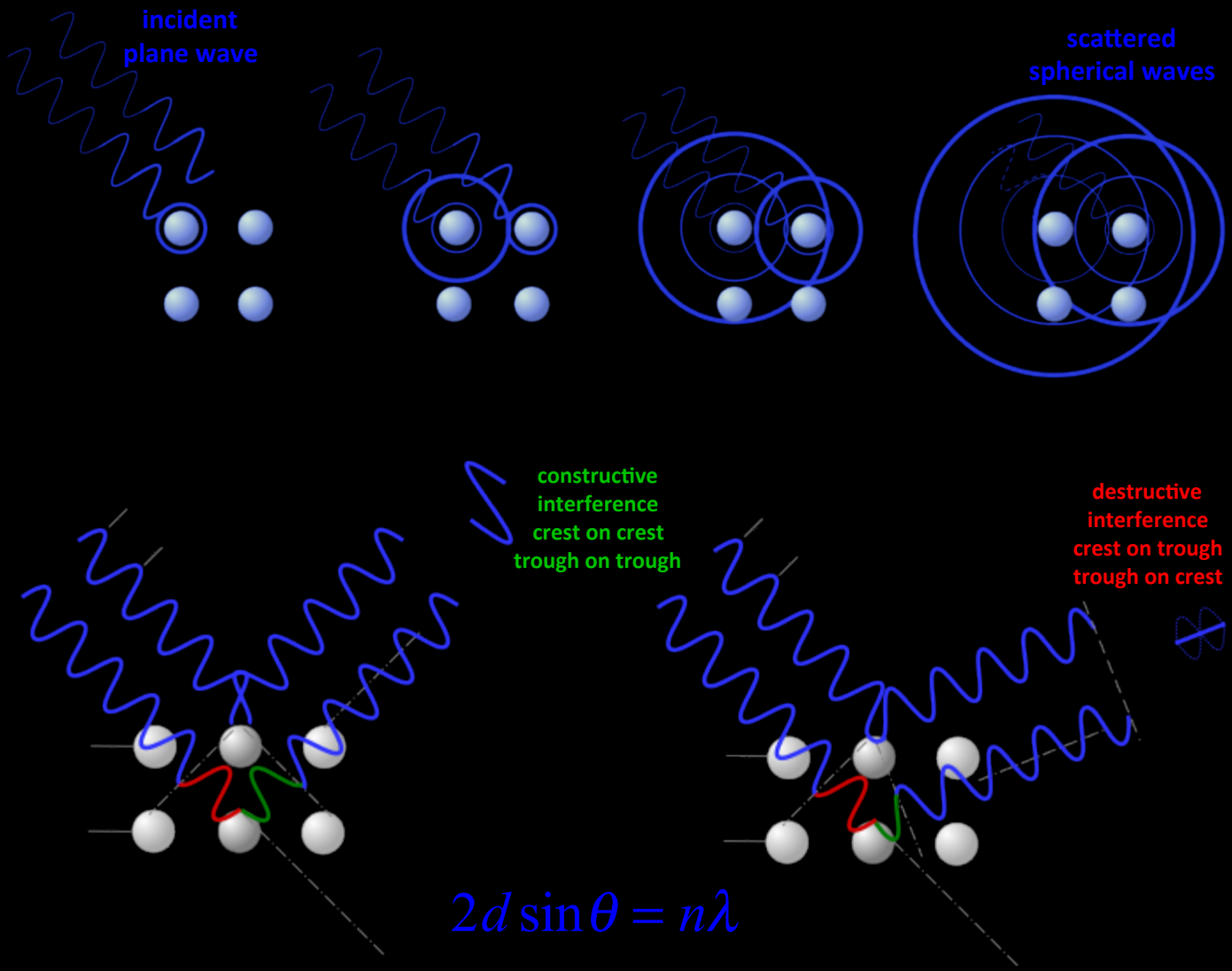
Thomson scattering of an X-ray wave due to driven oscillation of an electron



Elastic scattering of an electromagnetic wave

http://www.gly.uga.edu/schroeder/geol3010/3010lecture09.html

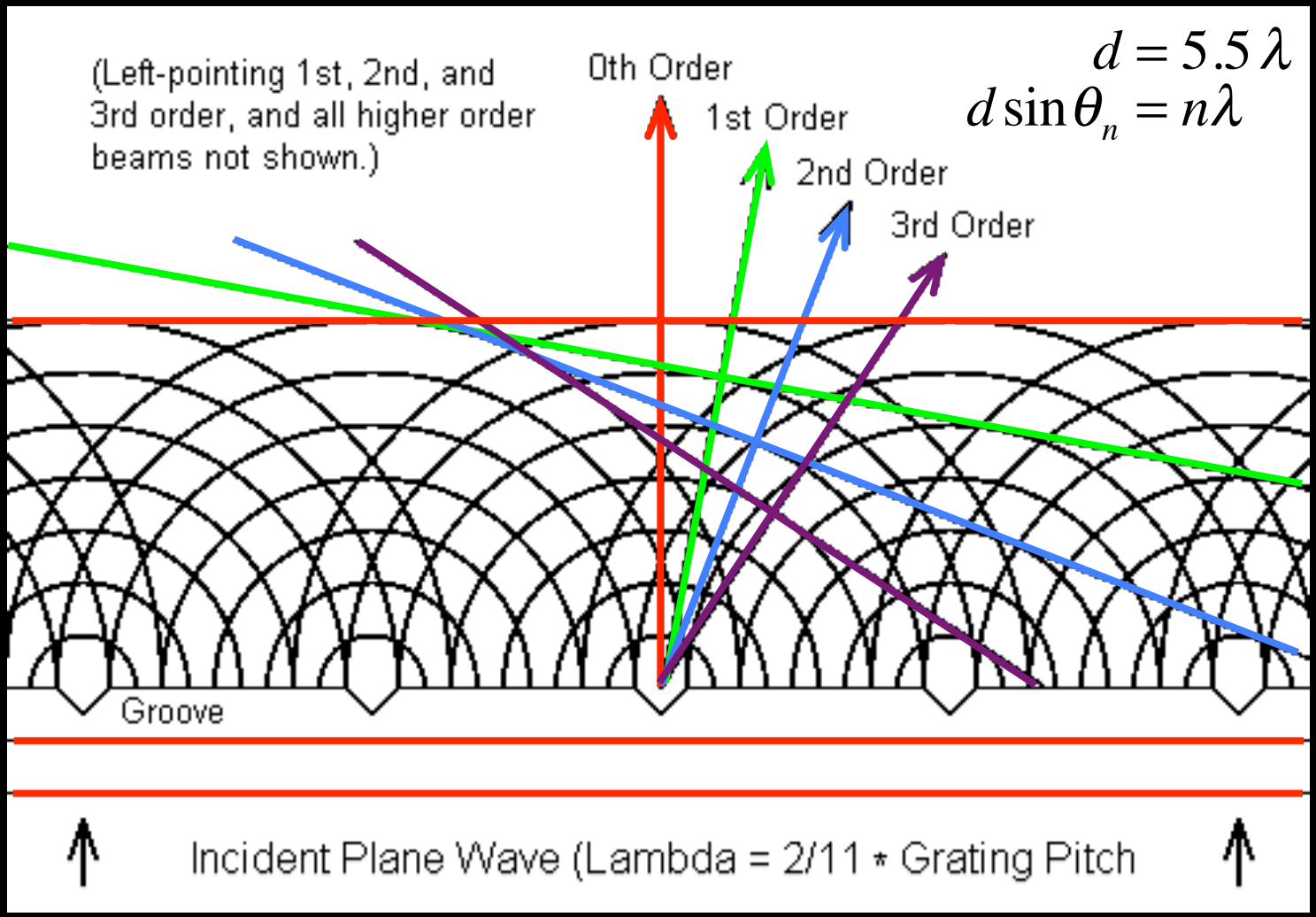
Rayleigh-Thomson scattering
Laue diffraction and Bragg reflection



Christophe Dang Ngoc Chan

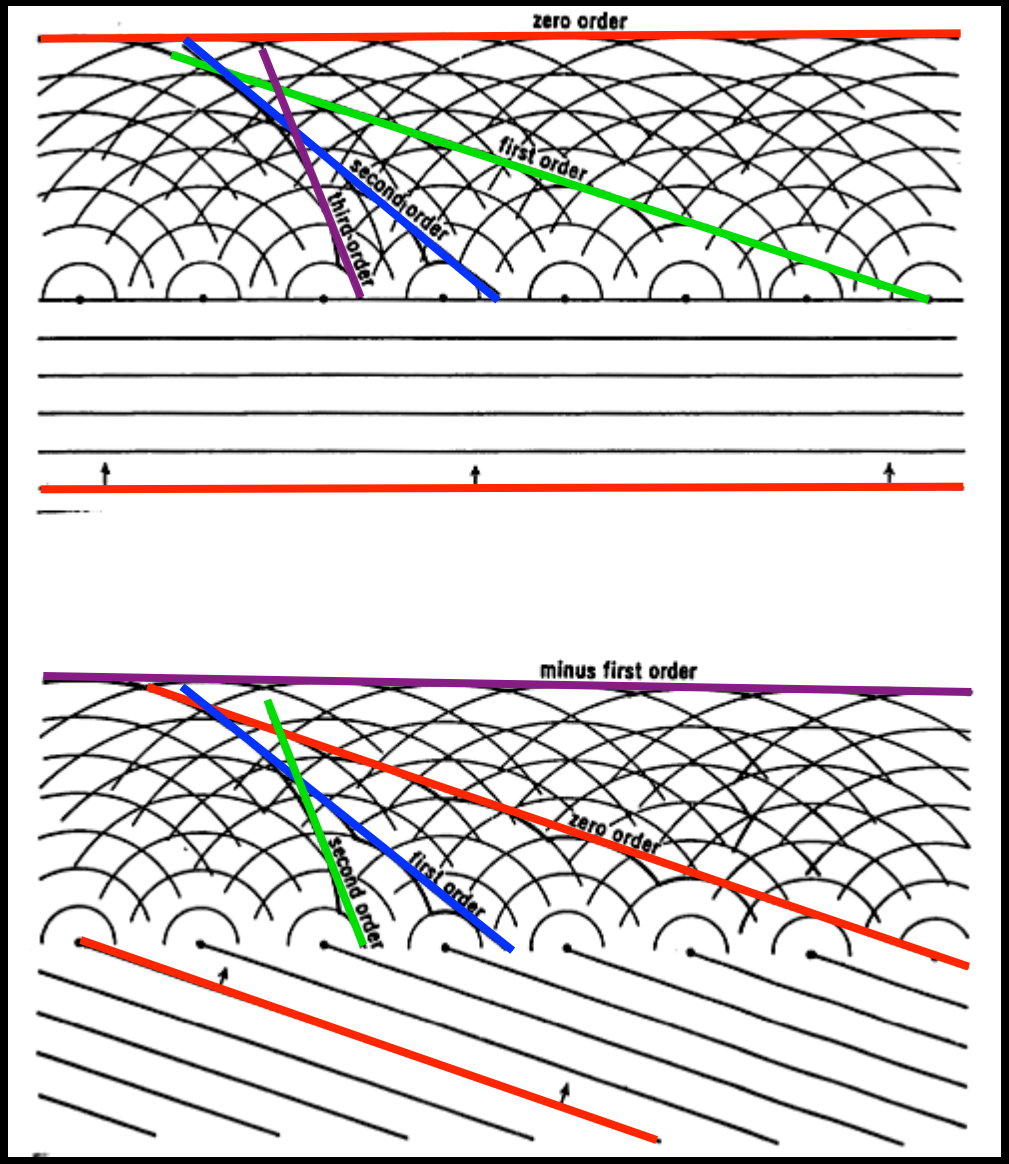
http://commons.wikimedia.org/wiki/File:Diffusion_rayleigh_et_diffraction.png
http://commons.wikimedia.org/wiki/File:Loi_de_bragg.png

Huygens construction for a diffraction grating with $d = 5.5\,\lambda$



http://www.eio.com/repairfaq/sam/diffract.gif

Huygens constructions for diffraction by a grating or by a lattice row



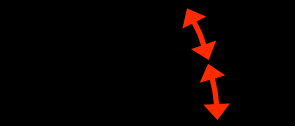
Martin J. Buerger (1962). *X-Ray Crystallography*. New York: John Wiley & Sons, Inc..

$\vec{a}$

$\vec{k}_0 + \vec{S} = \vec{k}$ $\quad \vec{S}$

$\vec{k} = \hat{s}/\lambda$

$\vec{\mathcal{E}} = \vec{\mathcal{E}}_0 e^{i(\omega t - \delta)}$



2θ

$\vec{k}_0 = \hat{s}_0/\lambda$

μ

ν

λ

$\vec{E} = \vec{E}_0 e^{i\omega t}$

$\hat{s}_0$ $\quad \hat{s}$

λ $\quad \vec{a}$ $\quad \hat{s}$

$\hat{s}_0$ $\quad \vec{a} \bullet \hat{s}$

$|\hat{s}_0| = |\hat{s}| = 1$

$\hat{s}_0 \bullet \hat{s} = \cos 2\theta$

$\vec{S} = \vec{k} - \vec{k}_0 = \dfrac{\hat{s} - \hat{s}_0}{\lambda}$

$|\vec{S}| = 2\left(\dfrac{\sin\theta}{\lambda}\right)$

$\text{path } 2 = |\hat{s}_0| + \vec{a} \bullet \hat{s}_0 + |\hat{s}|$

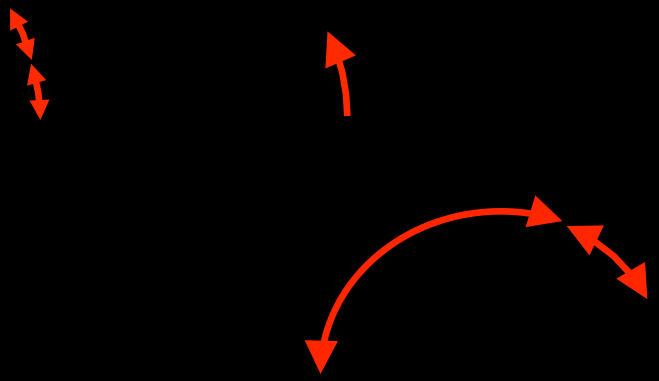
$\text{path } 1 - \text{path } 2 = \vec{a} \bullet \hat{s} - \vec{a} \bullet \hat{s}_0 = \vec{a} \bullet (\hat{s} - \hat{s}_0)$

$\vec{a} \bullet \hat{s}_0 = |\vec{a}| \cos\mu$

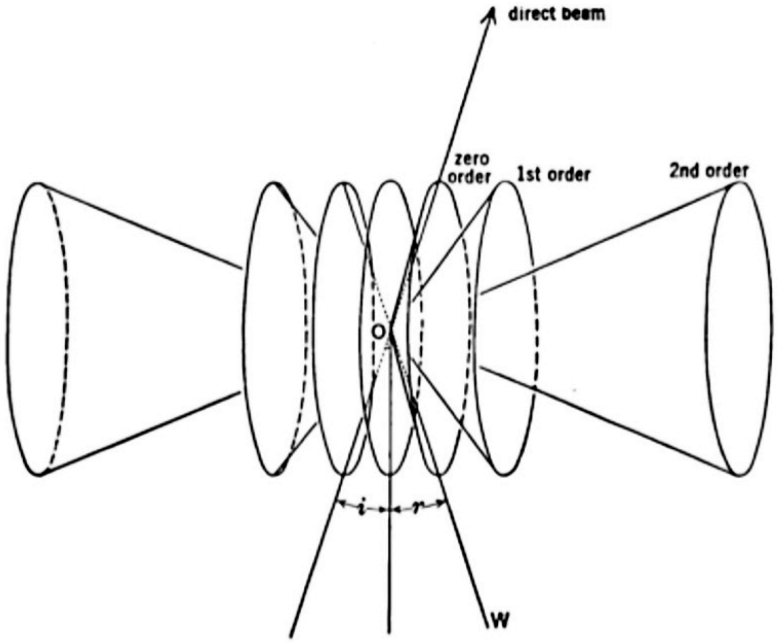
$\vec{a} \bullet \hat{s} = |\vec{a}| \cos\nu$

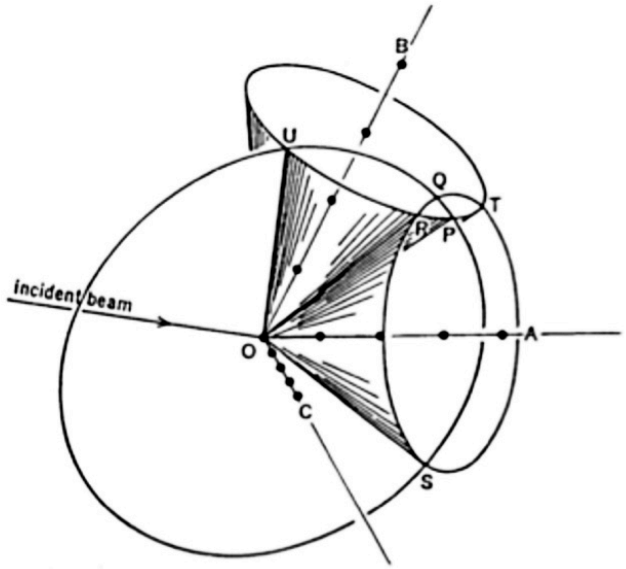
Laue diffraction condition

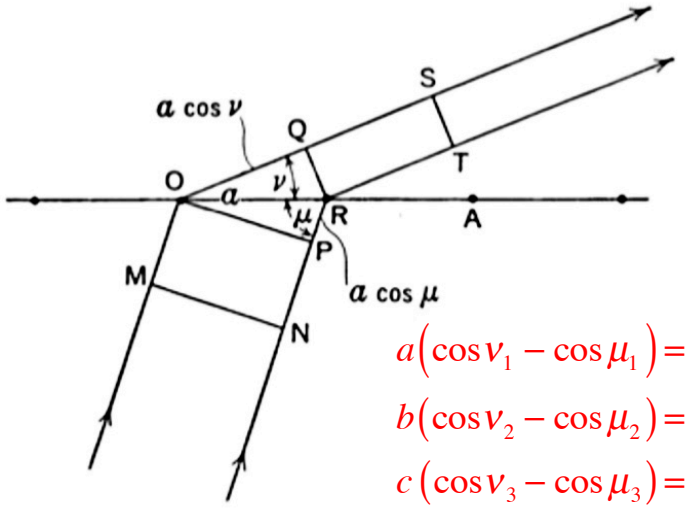
$\vec{a} \bullet (\hat{s} - \hat{s}_0) = |\vec{a}|(\cos\nu - \cos\mu) = h\lambda$

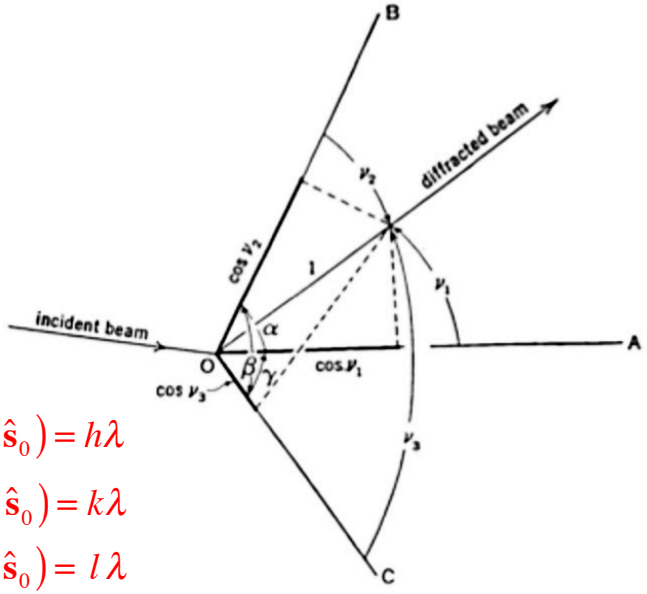


Laue diffraction by a three-dimensional lattice grating









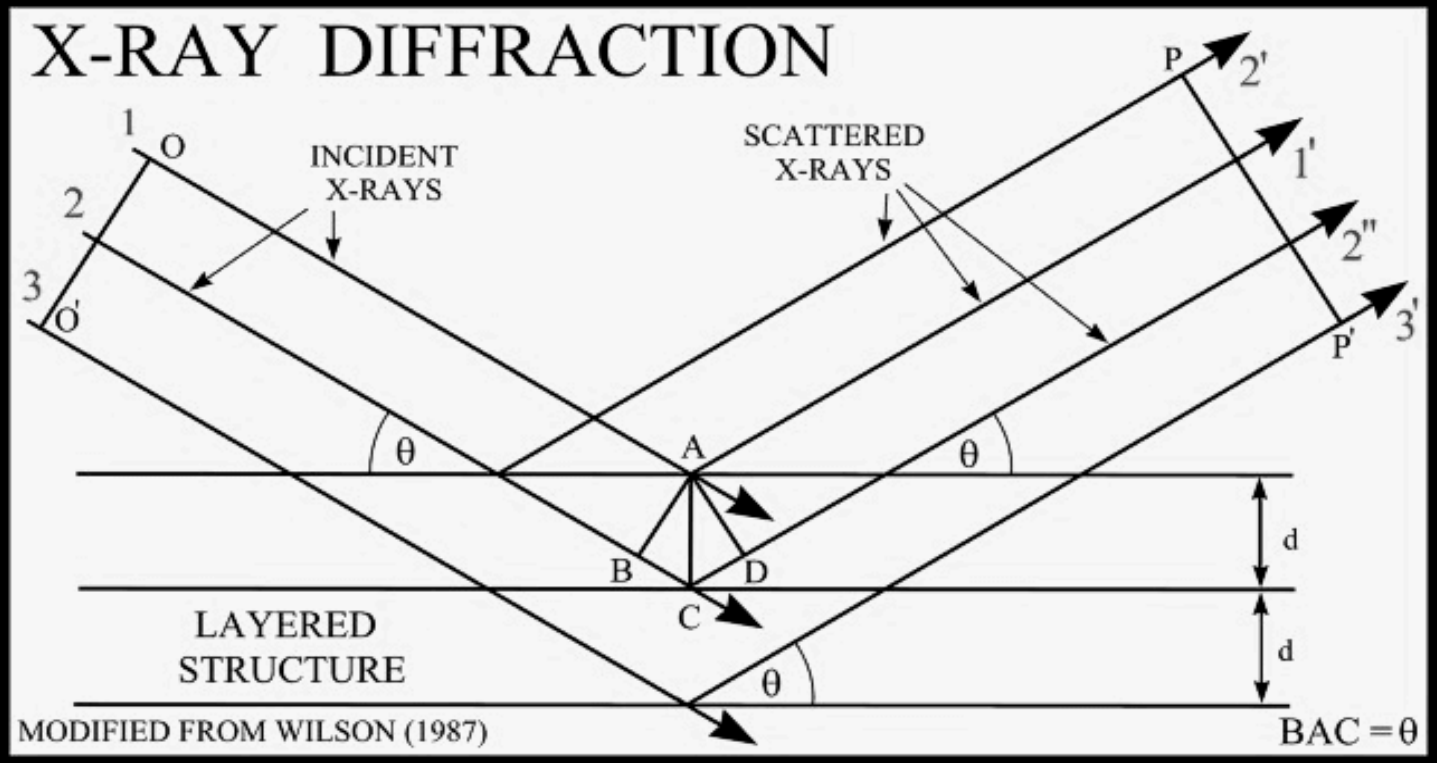
$$a\left(\cos\nu_1 - \cos\mu_1\right) = \mathbf{a}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = h\lambda$$

$$b\left(\cos\nu_2 - \cos\mu_2\right) = \mathbf{b}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = k\lambda$$

$$c\left(\cos\nu_3 - \cos\mu_3\right) = \mathbf{c}\bullet\left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right) = l\lambda$$

Martin J. Buerger (1962). *X-Ray Crystallography*. New York: John Wiley & Sons, Inc.

The Bragg Law $2d\sin\theta = n\lambda$



$$\measuredangle ABC = \measuredangle ADC = 90°$$

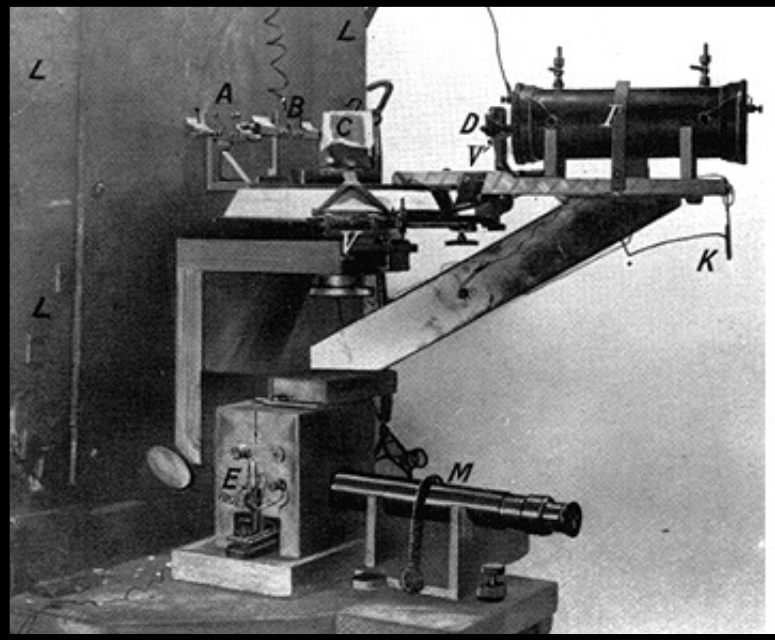
$$\measuredangle ACB = \measuredangle ADB = 90° - \theta$$

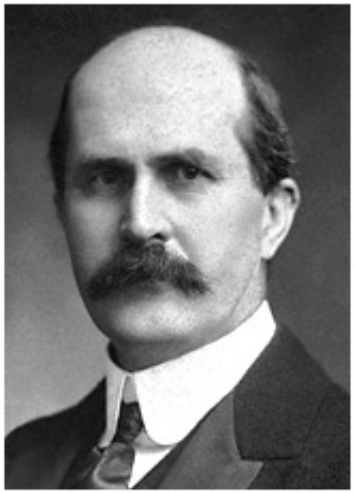
$$\measuredangle BAC = \measuredangle DAC = \theta$$

$$AC = d$$

$$BC = DC = d\sin\theta$$

http://pubs.usgs.gov/of/2001/of01-041/htmldocs/images/beam.jpg

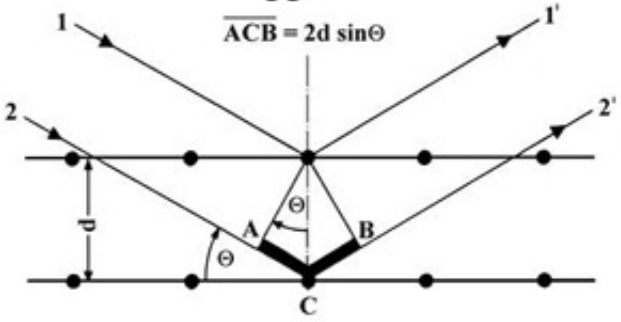


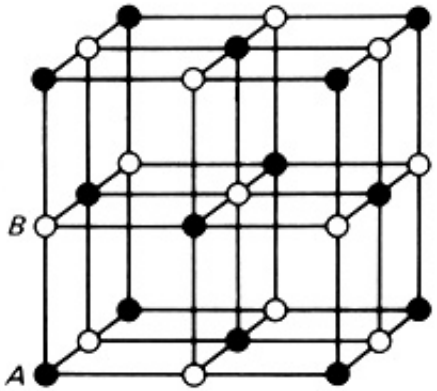


William Henry Bragg

Bragg's Law

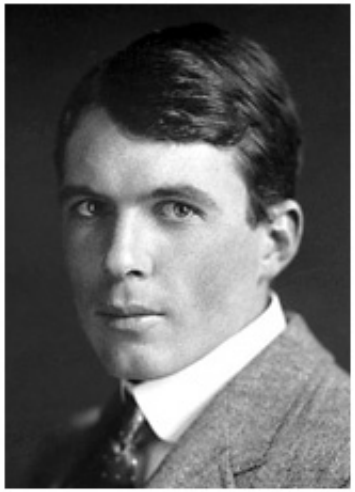
$\overline{ACB} = 2d \sin\Theta$





For NaCl

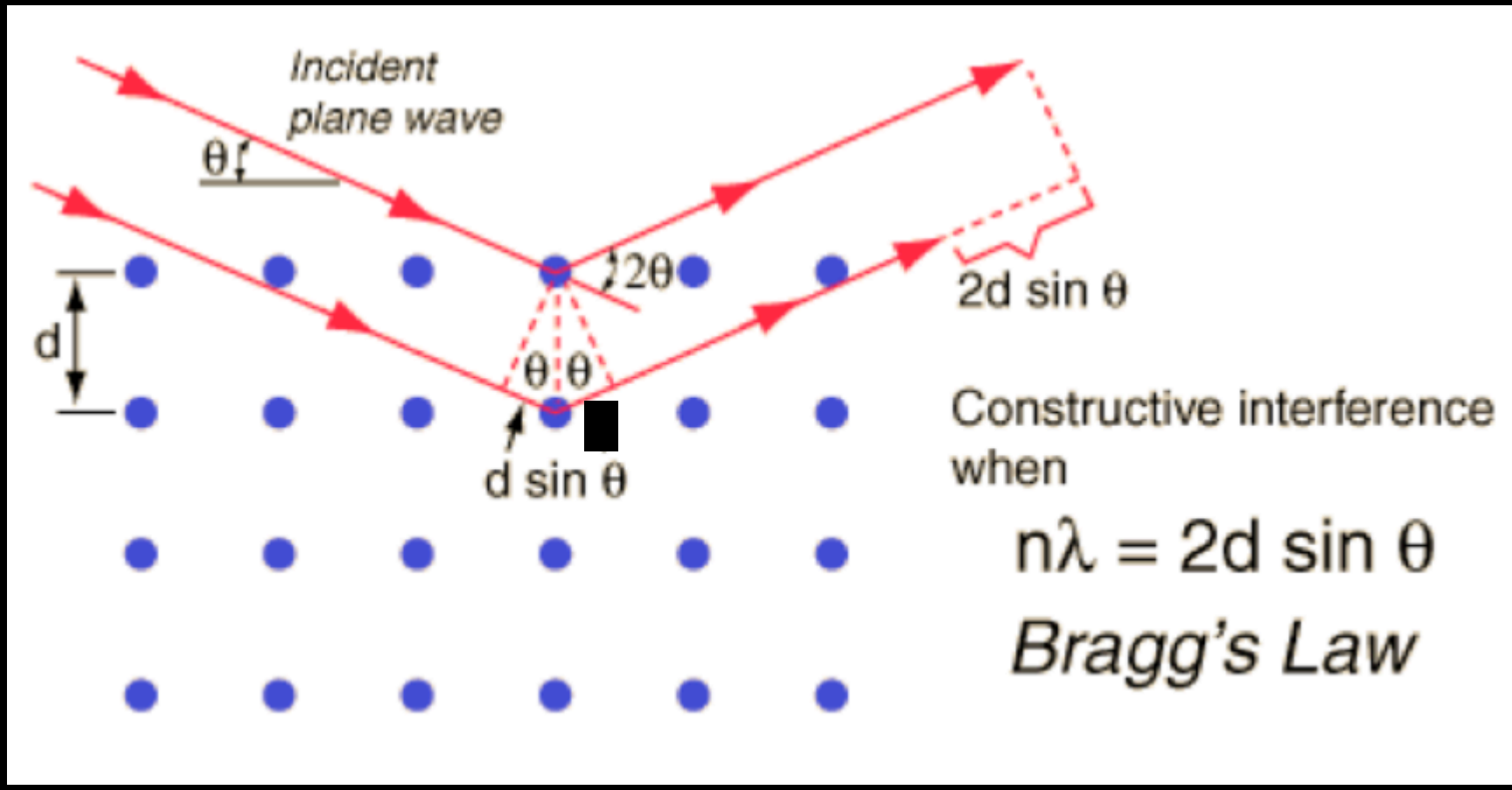
$AB = 2{\cdot}8 \times 10^{-8}$ cm



William Lawrence Bragg

http://www.diamond.ac.uk/Home/News/LatestNews/02-09-14.html

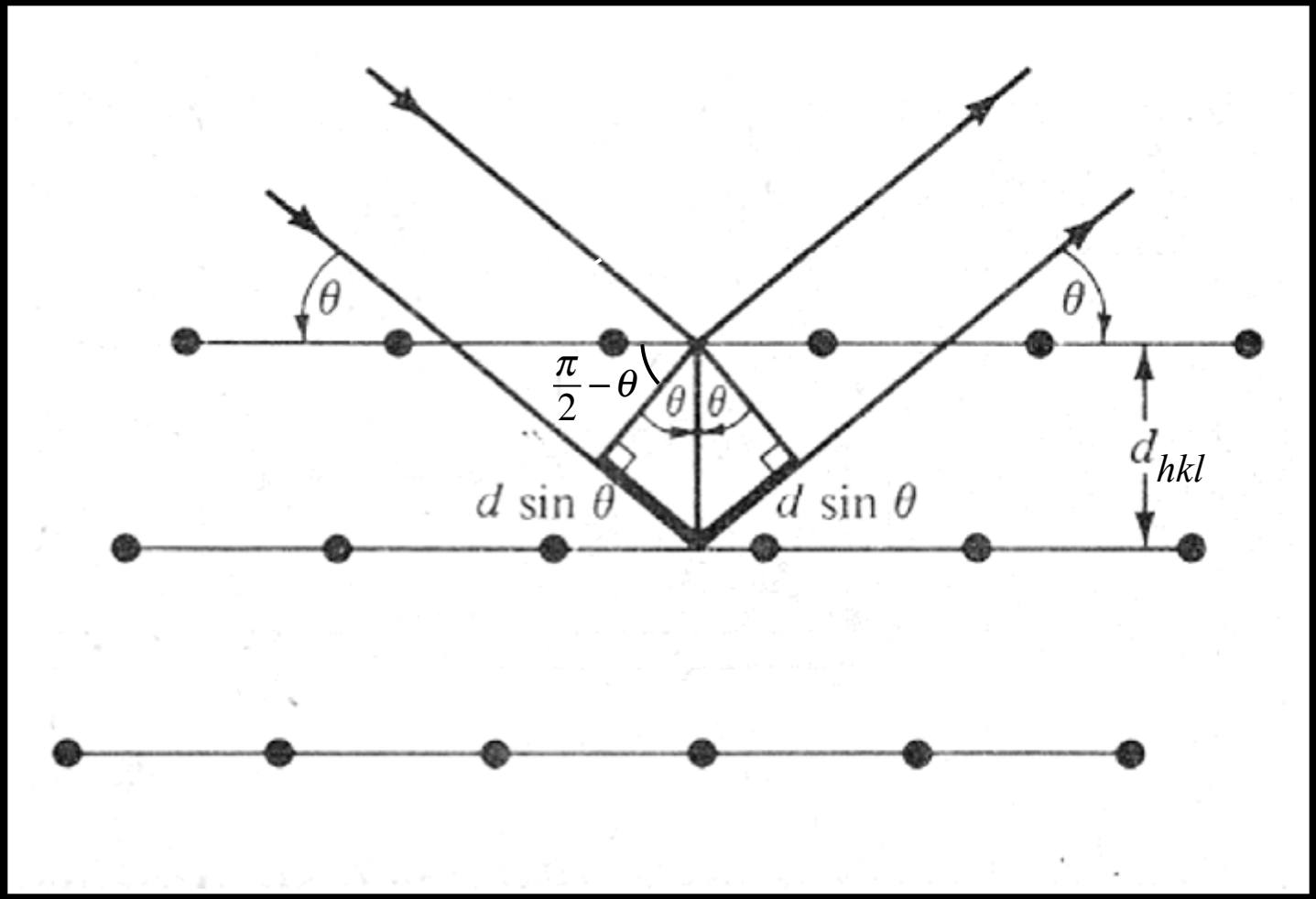
Bragg's law describes constructive interference of X-ray waves scattered by a crystal as specular reflection from families of parallel crystal lattice planes



http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/bragg.html

Bragg reflection from families of parallel *hkl* lattice planes

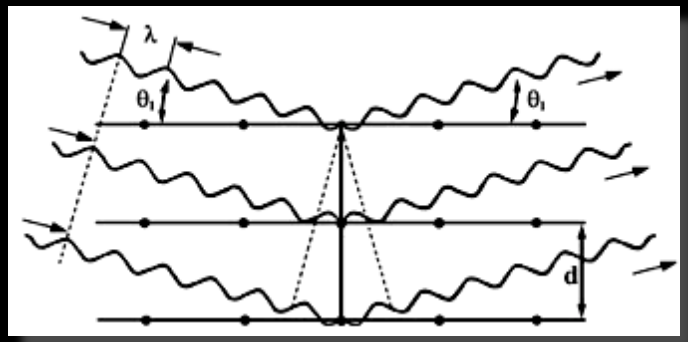
$$2d_{hkl}\sin\theta = n\lambda\,, \quad 2\left(\frac{d_{hkl}}{n}\right)\sin\theta = \lambda\,, \quad 2d_{nh\,nk\,nl}\sin\theta = \lambda$$



http://www.phy.ntnu.edu.tw/~changmc/Teach/SS/SSGI.htm

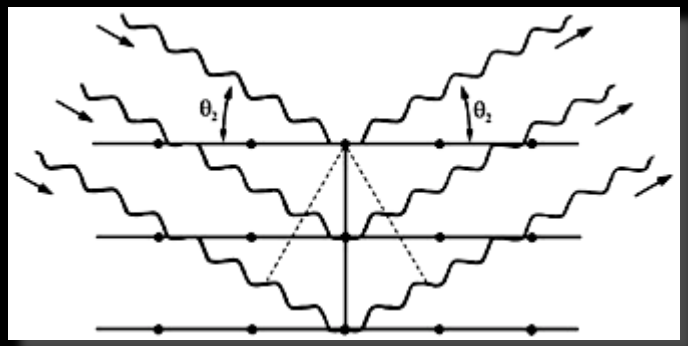
Orders of Bragg reflection from a family of parallel *hkl* lattice planes

1st order



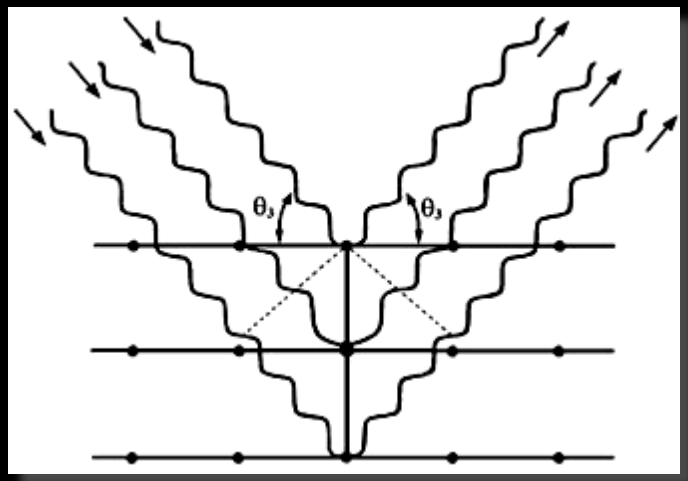
$$2d\sin\theta_1 = \lambda$$

2nd order



$$2d\sin\theta_2 = 2\lambda$$

3rd order

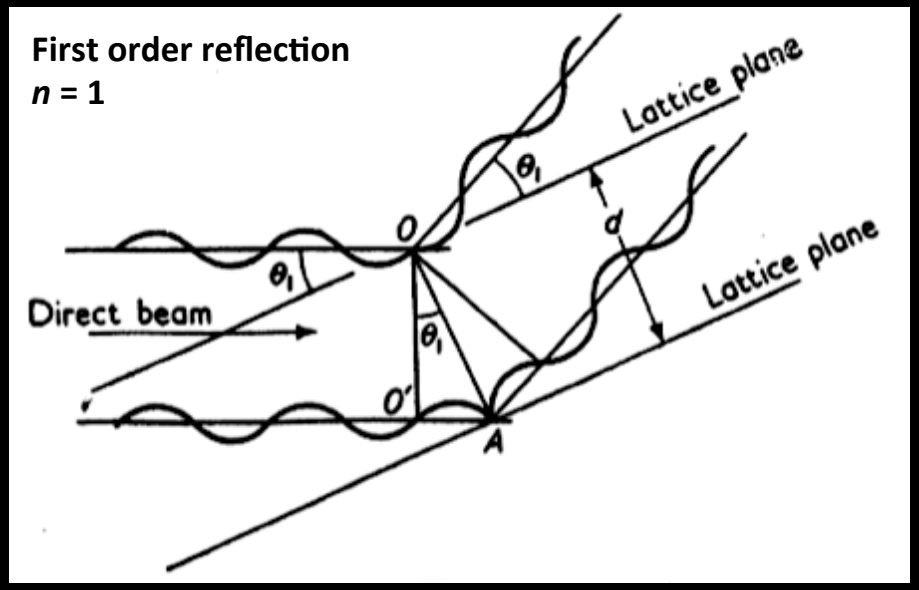


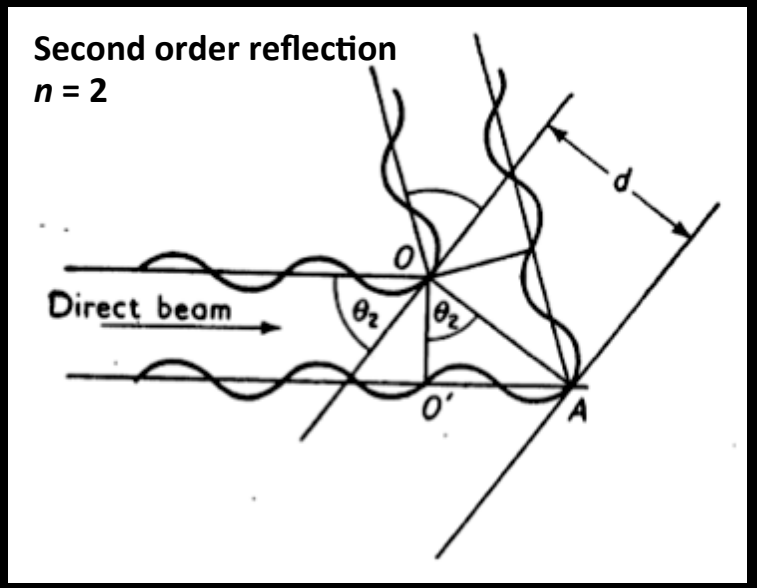
$$2d\sin\theta_3 = 3\lambda$$

http://www.bruker-axs.de/fileadmin/user_upload/xrfintro/sec1_8.html

Bragg reflections from a family of parallel *hkl* lattice planes

$$2d_{hkl}\sin\theta = n\lambda\,, \quad 2\left(\frac{d_{hkl}}{n}\right)\sin\theta = \lambda\,, \quad 2d_{nh\,nk\,nl}\sin\theta = \lambda$$





$$2d_{hkl}\sin\theta_1 = \lambda$$

$$2d_{hkl}\sin\theta_2 = 2\lambda$$

$$2\left(\frac{d_{hkl}}{2}\right)\sin\theta_2 = \lambda$$

$$2d_{2h\,2k\,2l}\sin\theta_2 = \lambda$$

Monochromatic X-ray diffraction

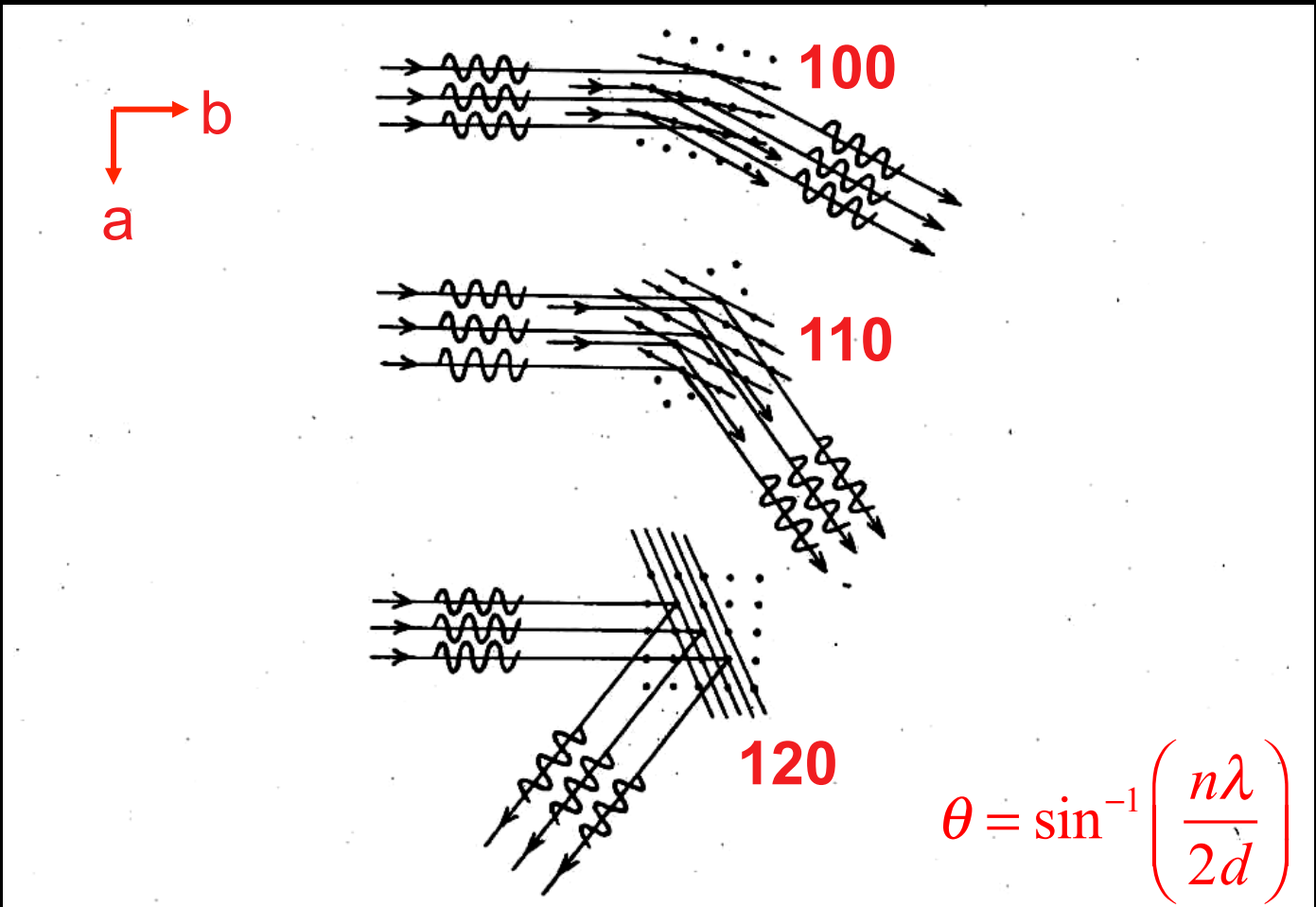


FIG. 113. When a crystal is rotated in a monochromatic X-ray beam, the various planes of atoms are able to reflect only at particular angles; the angle at which reflection takes place depends on the spacing of the planes. The more widely spaced planes give reflections near the primary beam; the more closely spaced planes reflect at the larger angles.

Charles W. Bunn (1964). *Crystals: Their Role in Nature and in Science*. New York: Academic Press

Polychromatic X-ray diffraction

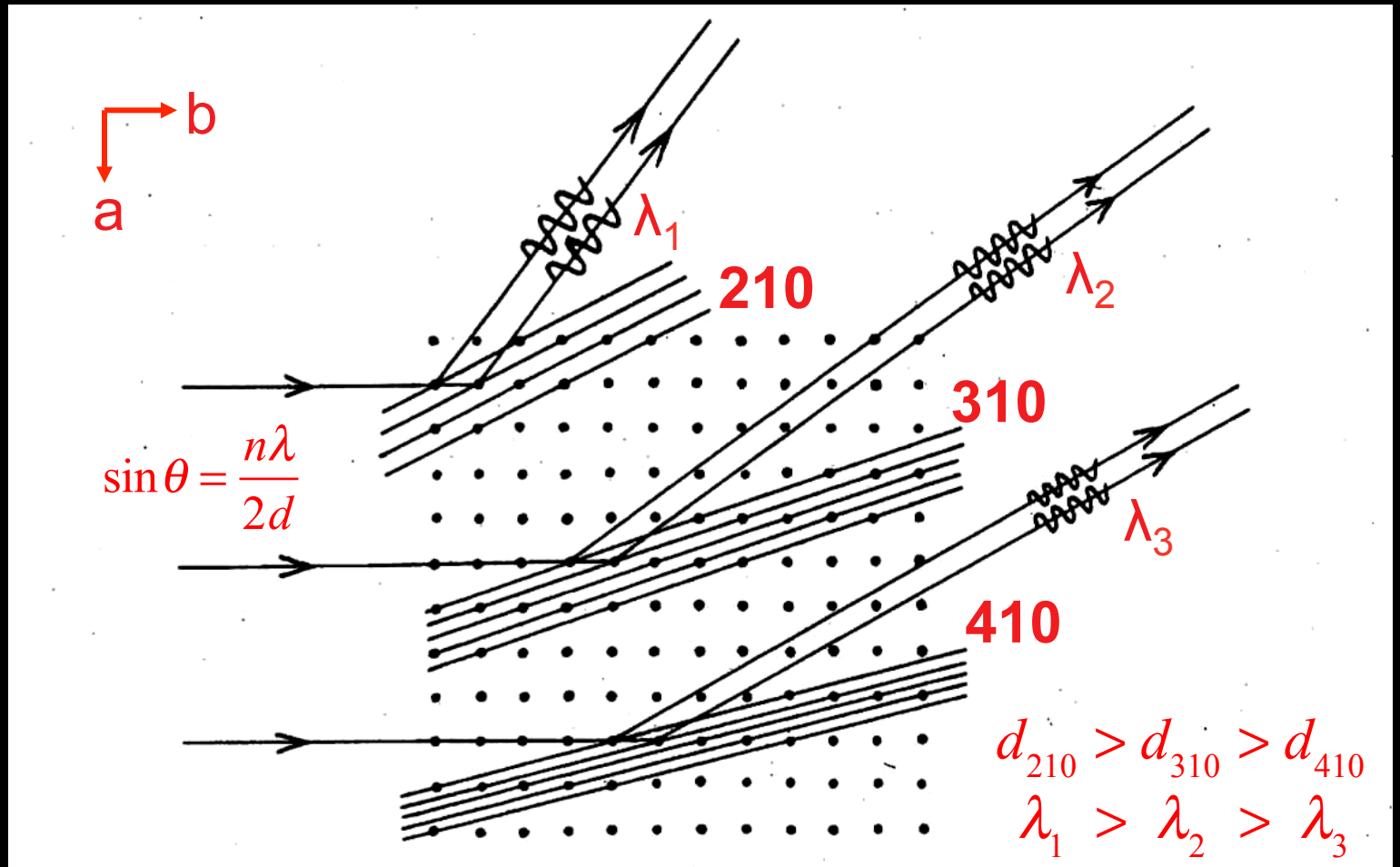


FIG. 111. In Laue's experiment, each spot on the plate is due to the reflection of X-rays by a different set of atomic planes acting as X-ray mirrors. The more widely spaced planes reflect the longer waves in the beam, while the more closely spaced planes reflect the shorter waves, at smaller angles.

Charles W. Bunn (1964). *Crystals: Their Role in Nature and in Science*. New York: Academic Press

Polychromatic X-ray diffraction

According to the Bragg law $2d_{hkl} \sin \theta_{hkl} = \lambda$, the discrete lattice spacings d_{hkl} select discrete monochromatic wavelengths $\lambda_i = 2d_{hkl} (\sin \theta_{hkl})$ from a polychromatic X-ray beam.

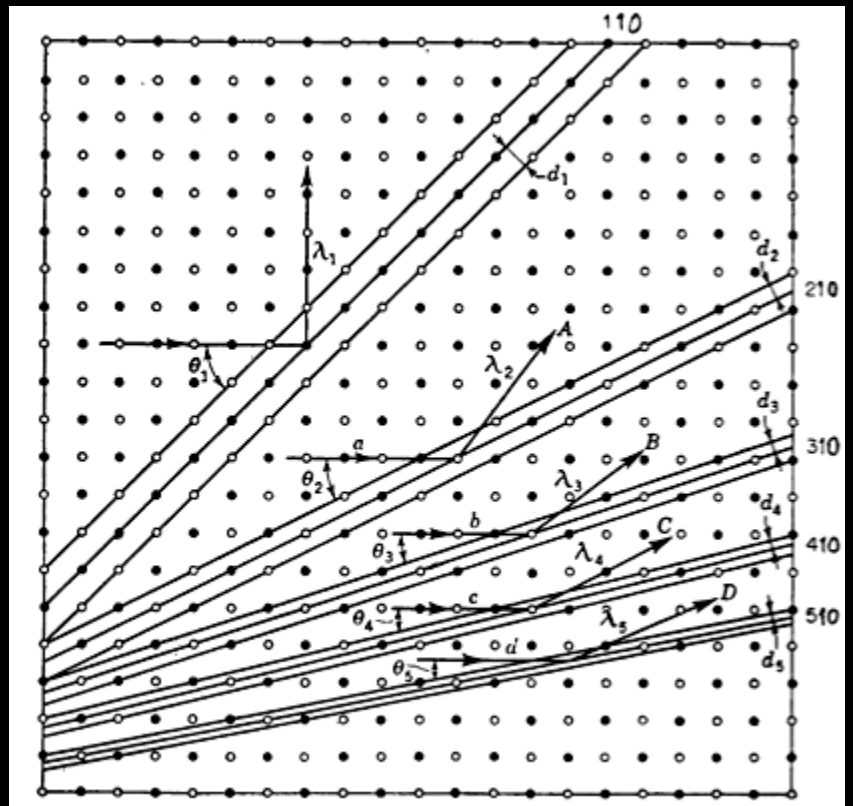


FIG. 129. Schematic representation of the reflection of monochromatic beams of x-rays by a crystal of NaCl when a heterochromatic beam is incident upon it.

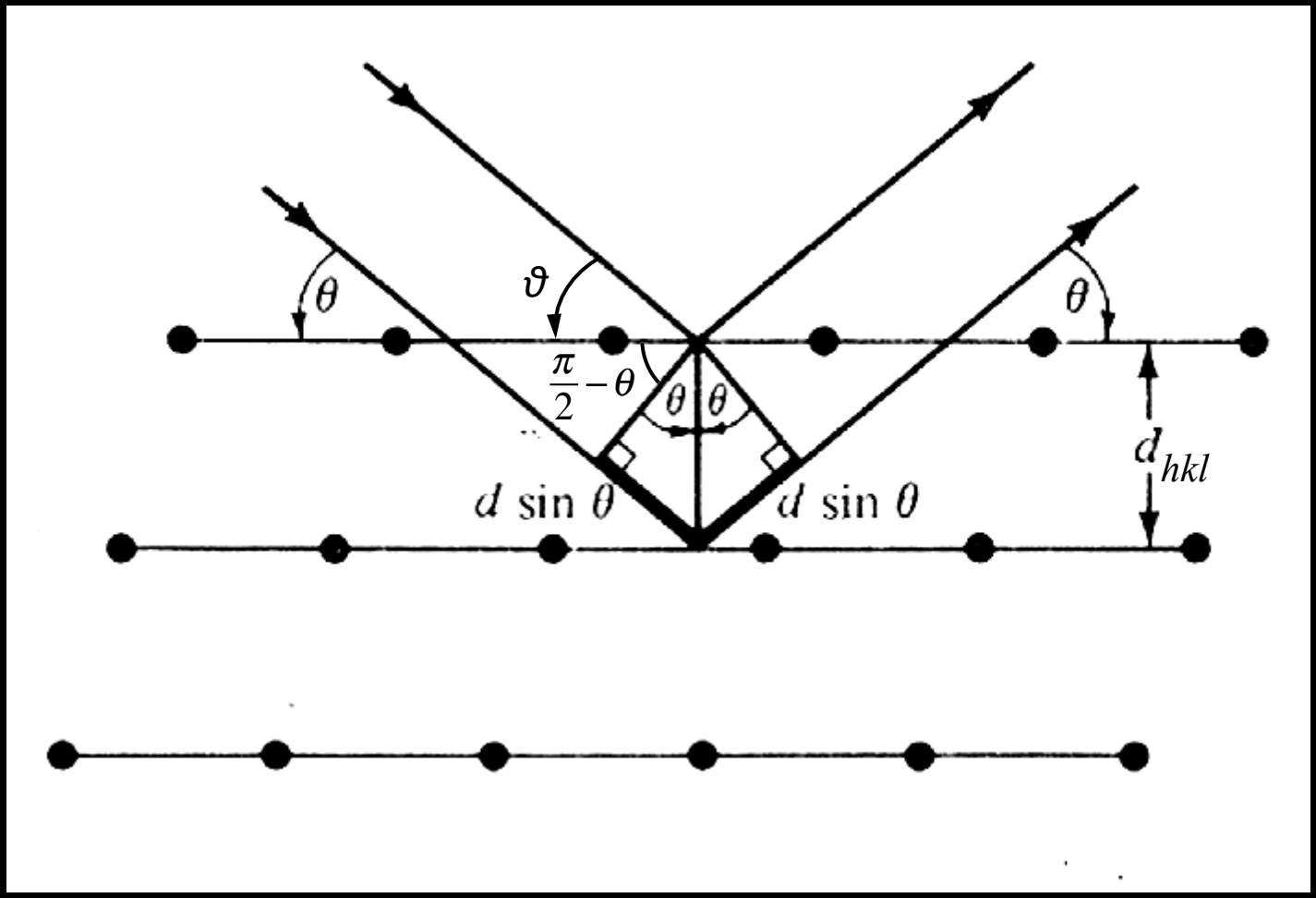
$$d_{110} > d_{210} > d_{310} > d_{410} > d_{510}$$

$$\theta_1 > \theta_2 > \theta_3 > \theta_4 > \theta_5$$

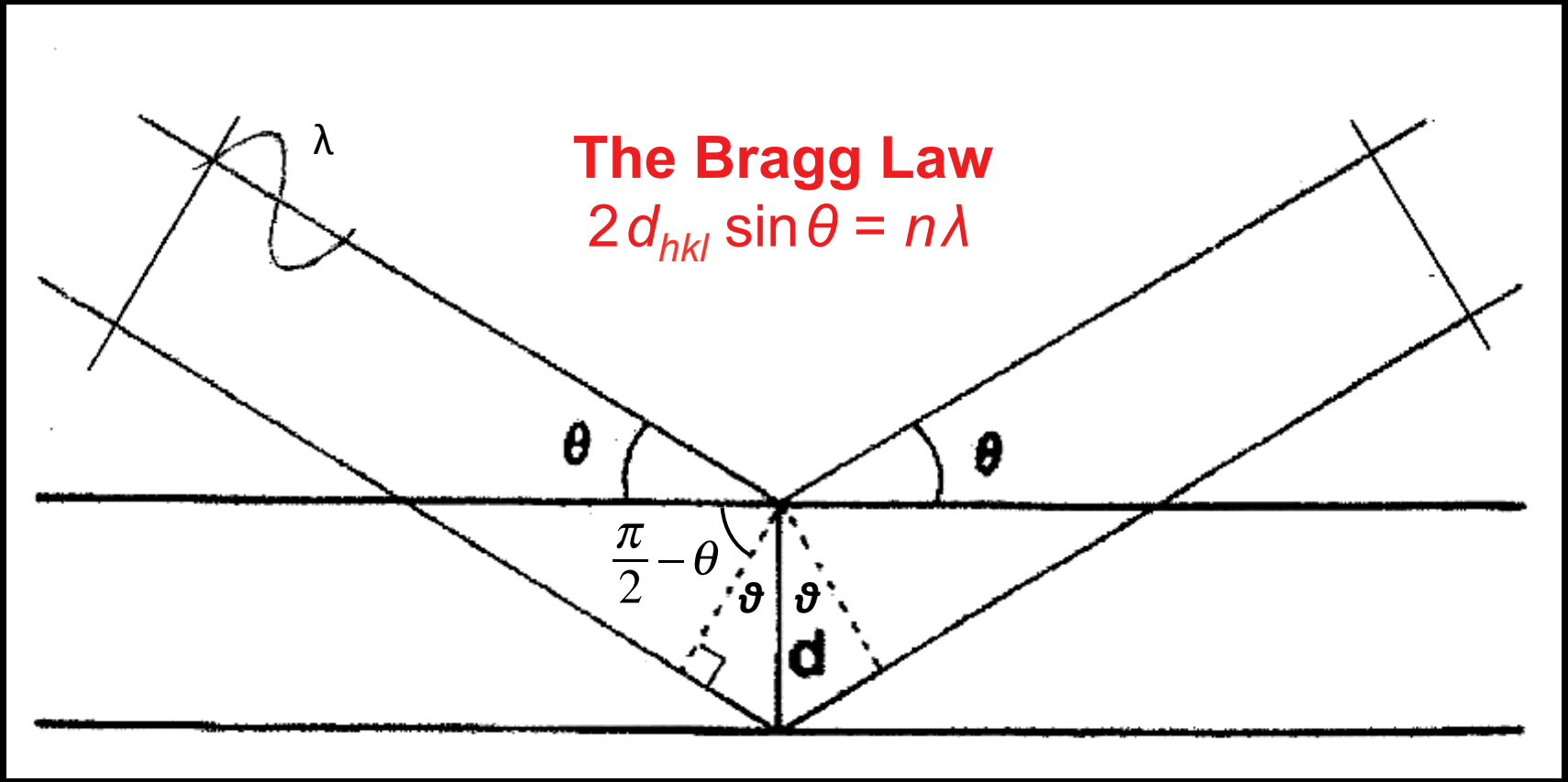
$$\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 > \lambda_5$$

Bragg reflection from families of parallel *hkl* lattice planes

$$2d_{hkl}\sin\theta = n\lambda\,, \qquad 2\left(\frac{d_{hkl}}{n}\right)\sin\theta = \lambda\,, \qquad 2d_{nh\,nk\,nl}\sin\theta = \lambda$$

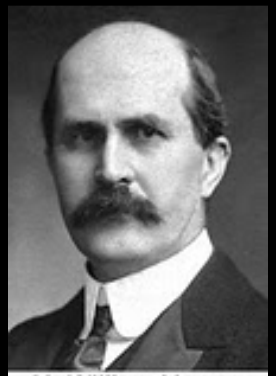


http://www.phy.ntnu.edu.tw/~changmc/Teach/SS/SSGI.htm



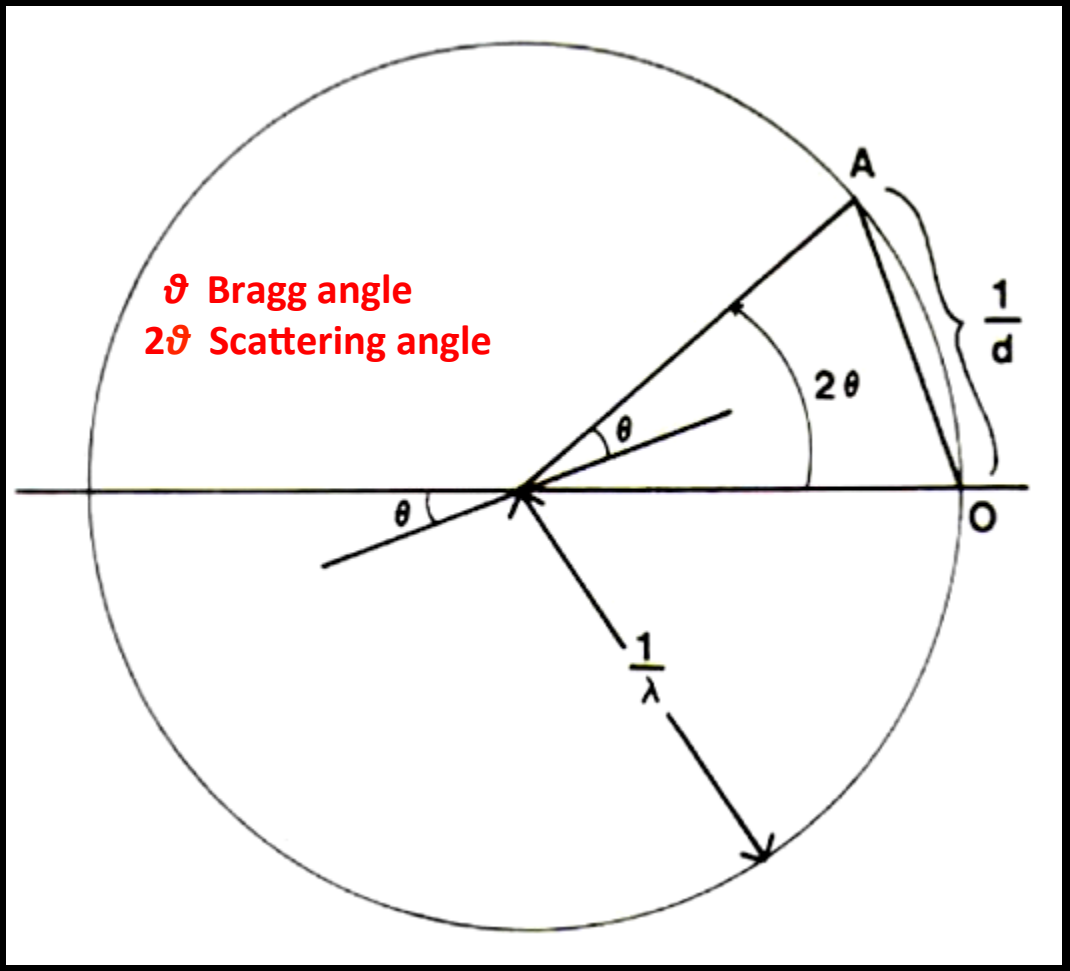
Robert M.Sweet (1985). Introduction to Crystallography. In *Methods in Enzymology*, v.114.

The Ewald construction for the Bragg reflection law



Sir William Henry Bragg
(1862 - 1942)

William Lawrence Bragg
(1890 - 1971)



Paul Peter Ewald
1888-1985

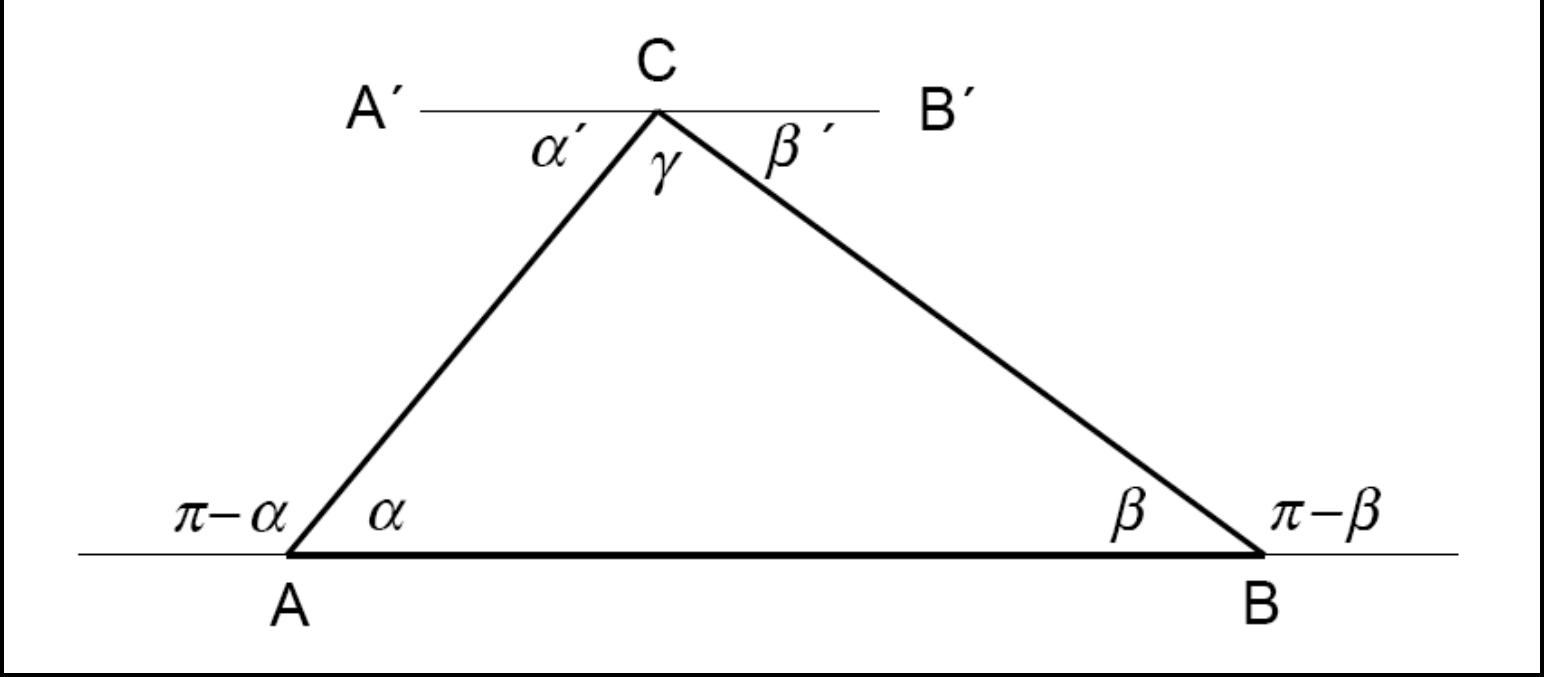
Wm. Henry & Wm. Lawrence Bragg (1913) $2d\sin\theta = \lambda$

Paul Peter Ewald (1913) $\sin\theta = \frac{1}{2}\frac{\lambda}{d} = \left(\frac{1}{d}\right)\Big/\left(\frac{2}{\lambda}\right)$

Robert M. Sweet (1985). Introduction to Crystallography. In *Methods in Enzymology*, v.114.

http://sandwalk.blogspot.com/2008/03/nobel-laureates-sir-william-henry-bragg.html

http://wwwuser.gwdg.de/~nprofwg/ForeignScientists.html



$A'B' \parallel AB$

$$\alpha' = \alpha$$

$$\beta' = \beta$$

$$\alpha' + \gamma + \beta' = \alpha + \beta + \gamma = \pi$$

$$\alpha + \beta + (\alpha + \beta) = \pi$$

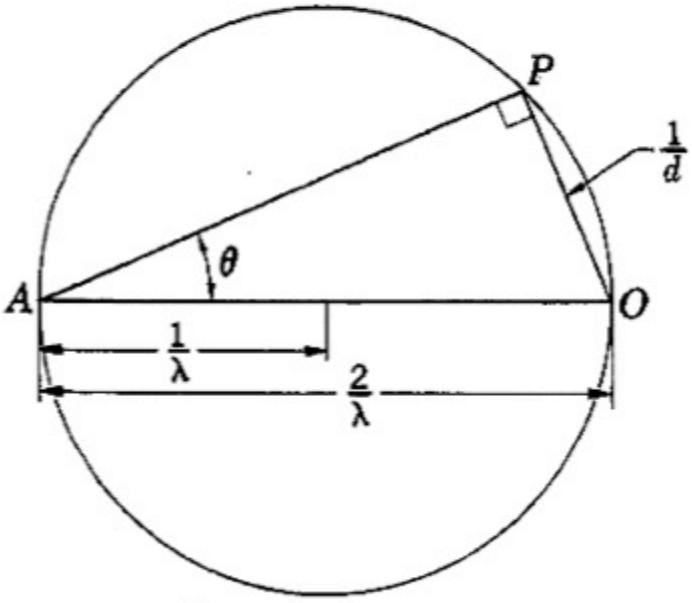
$$2\alpha + 2\beta = \pi$$

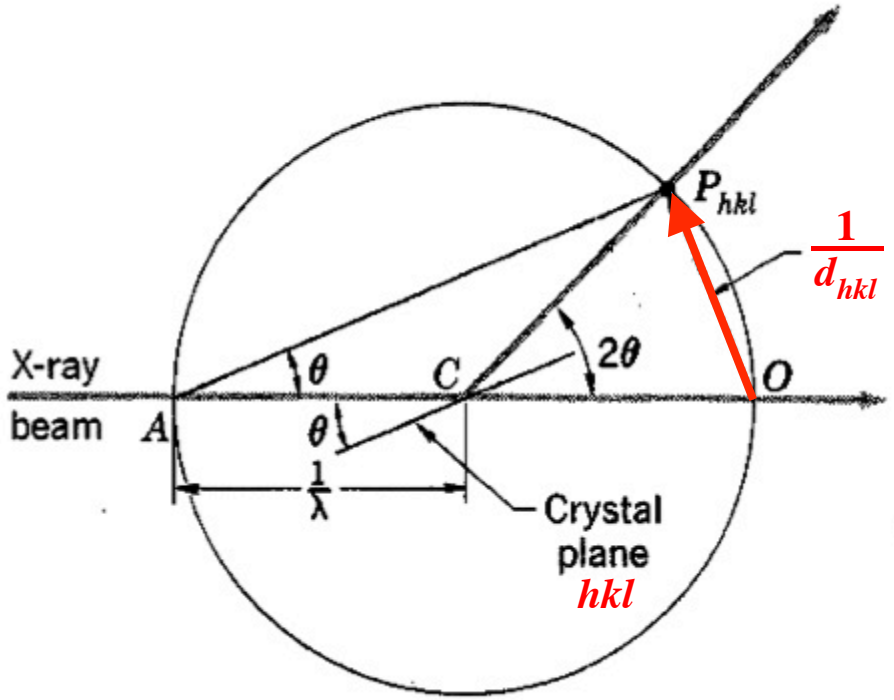
$$\alpha + \beta = \frac{\pi}{2}$$

The Ewald construction for the Bragg reflection law

ϑ Bragg angle

2ϑ Scattering angle





Wm. Henry & Wm. Lawrence Bragg (1913) $2d\sin\theta = \lambda$

Paul Peter Ewald (1913) $\sin\theta = \frac{1}{d}\frac{\lambda}{2} = \left(\frac{1}{d}\right)\Big/\left(\frac{2}{\lambda}\right)$

Leonid V. Azároff (1968). *Elements of X-ray Crystallography*. McGraw-Hill Book Co.

The Ewald construction for the Bragg reflection law

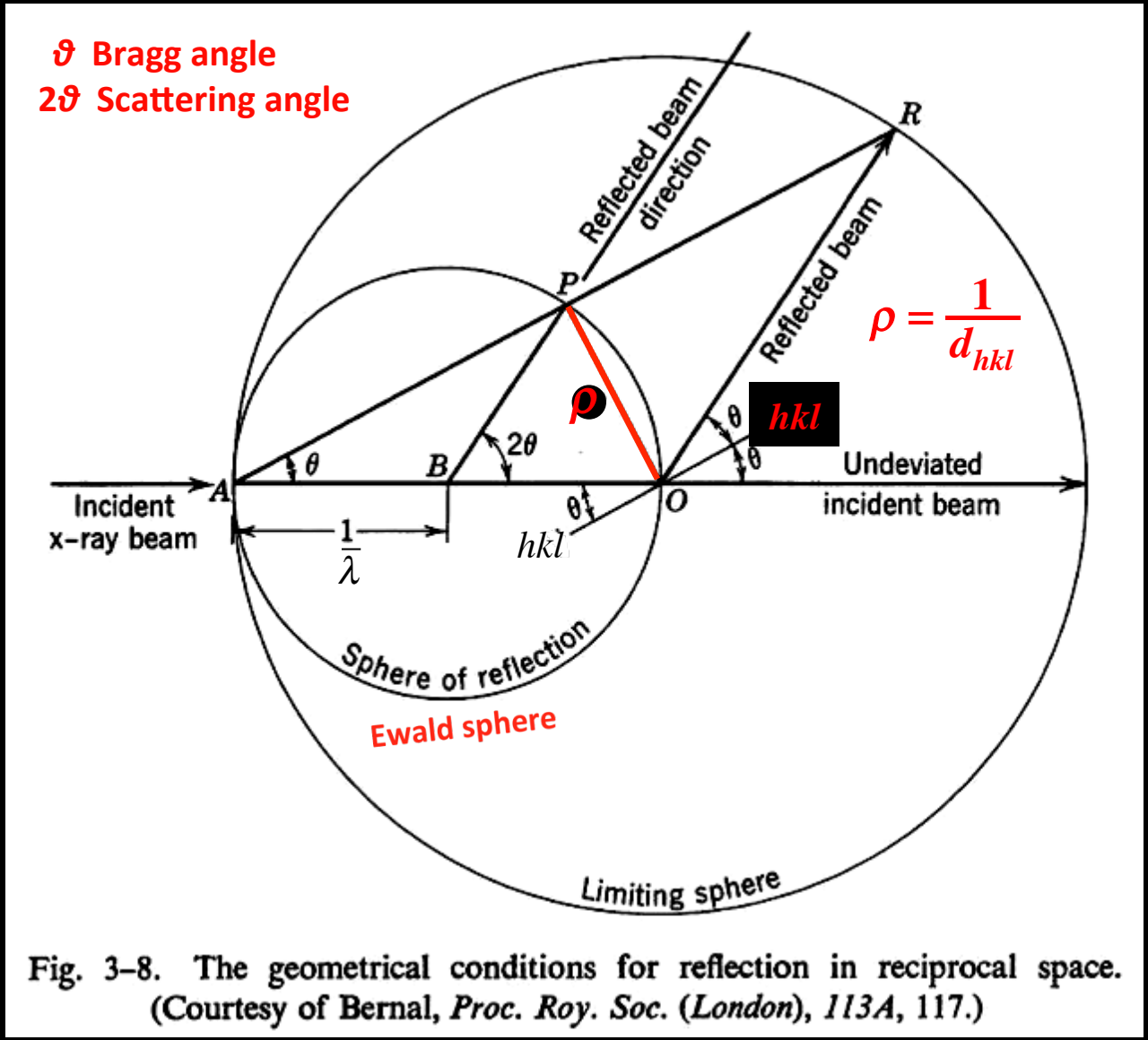


Fig. 3–8. The geometrical conditions for reflection in reciprocal space. (Courtesy of Bernal, *Proc. Roy. Soc.* (*London*), *113A*, 117.)

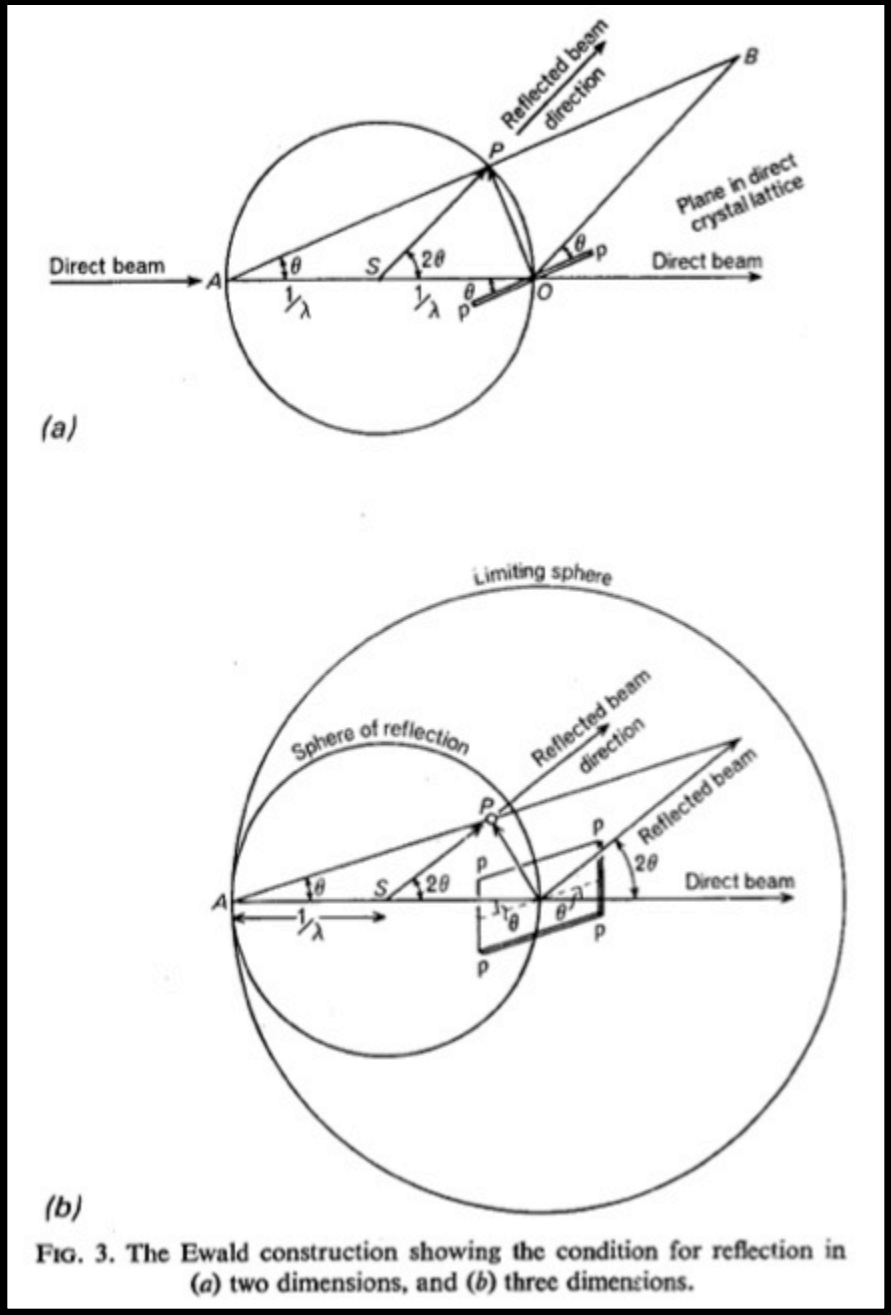


FIG. 3. The Ewald construction showing the condition for reflection in (*a*) two dimensions, and (*b*) three dimensions.

W.L. Bragg, *The Development of X-Ray Analysis* (revised edition). New York: Dover Publications, Inc., 1992.

The Ewald construction

$$2d_{hkl}\sin\theta_{hkl}=\lambda$$

$$\sin\theta_{hkl}=\frac{\lambda}{2d_{hkl}}=\frac{1}{2}\,\frac{1/d_{hkl}}{1/\lambda}=\frac{d^*_{hkl}}{2/\lambda}$$

$$\mathbf{H}=\frac{\hat{\mathbf{s}}-\hat{\mathbf{s}}_0}{\lambda}$$

$$\left|\mathbf{H}\right|=d^*_{hkl}=2\left(\frac{\sin\theta_{hkl}}{\lambda}\right)$$

$$\measuredangle\mathrm{AOX}=\pi-2\theta$$

$$\therefore\ \measuredangle\mathrm{OAX}=\measuredangle OXA=\theta$$

$$\measuredangle\mathrm{OXY}=\measuredangle\mathrm{OYX}=\frac{1}{2}(\pi-2\theta)=\frac{\pi}{2}-\theta$$

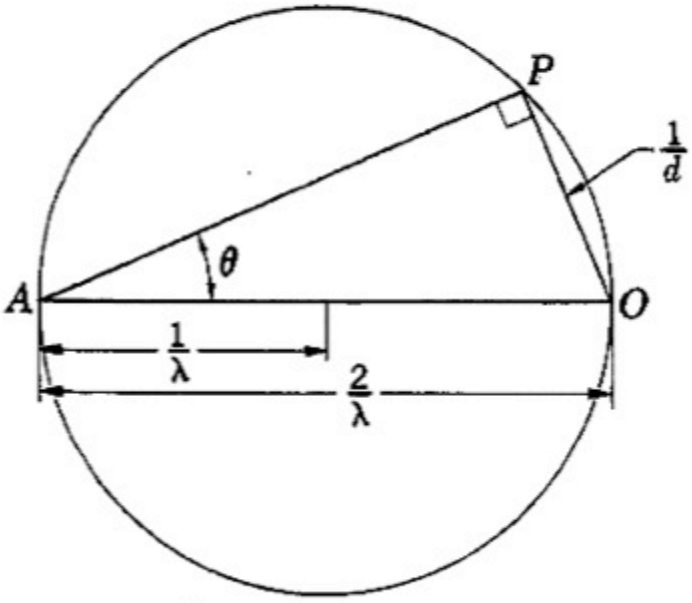
$$\therefore\ \measuredangle\mathrm{AXY}=\frac{\pi}{2}$$

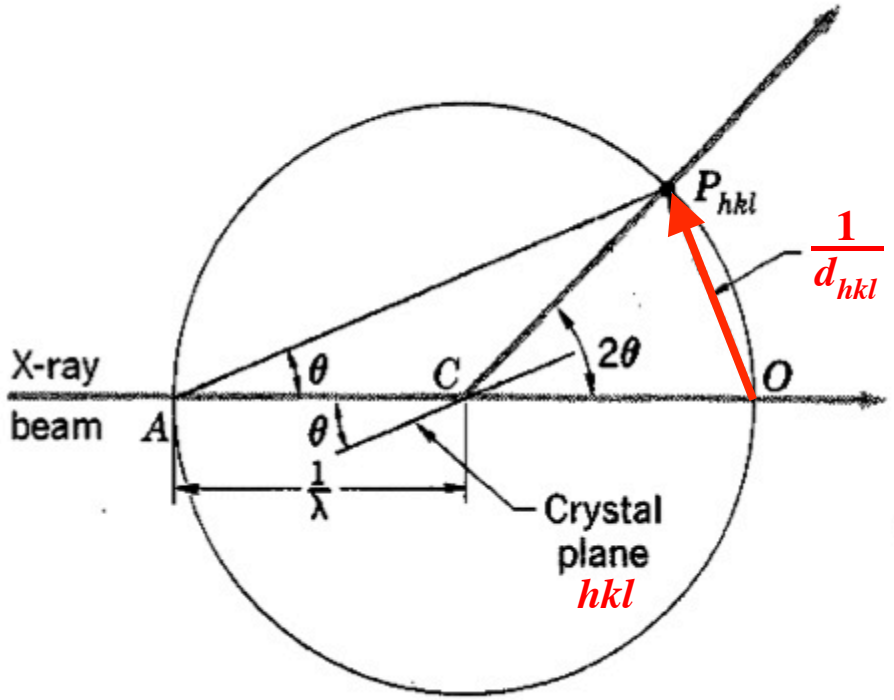
http://www.msm.cam.ac.uk/doitpoms/tlplib/xray-diffraction/ http://perso.fundp.ac.be/~jwouters/DRX/diffraction.html

The Ewald construction for the Bragg reflection law

ϑ Bragg angle

2ϑ Scattering angle



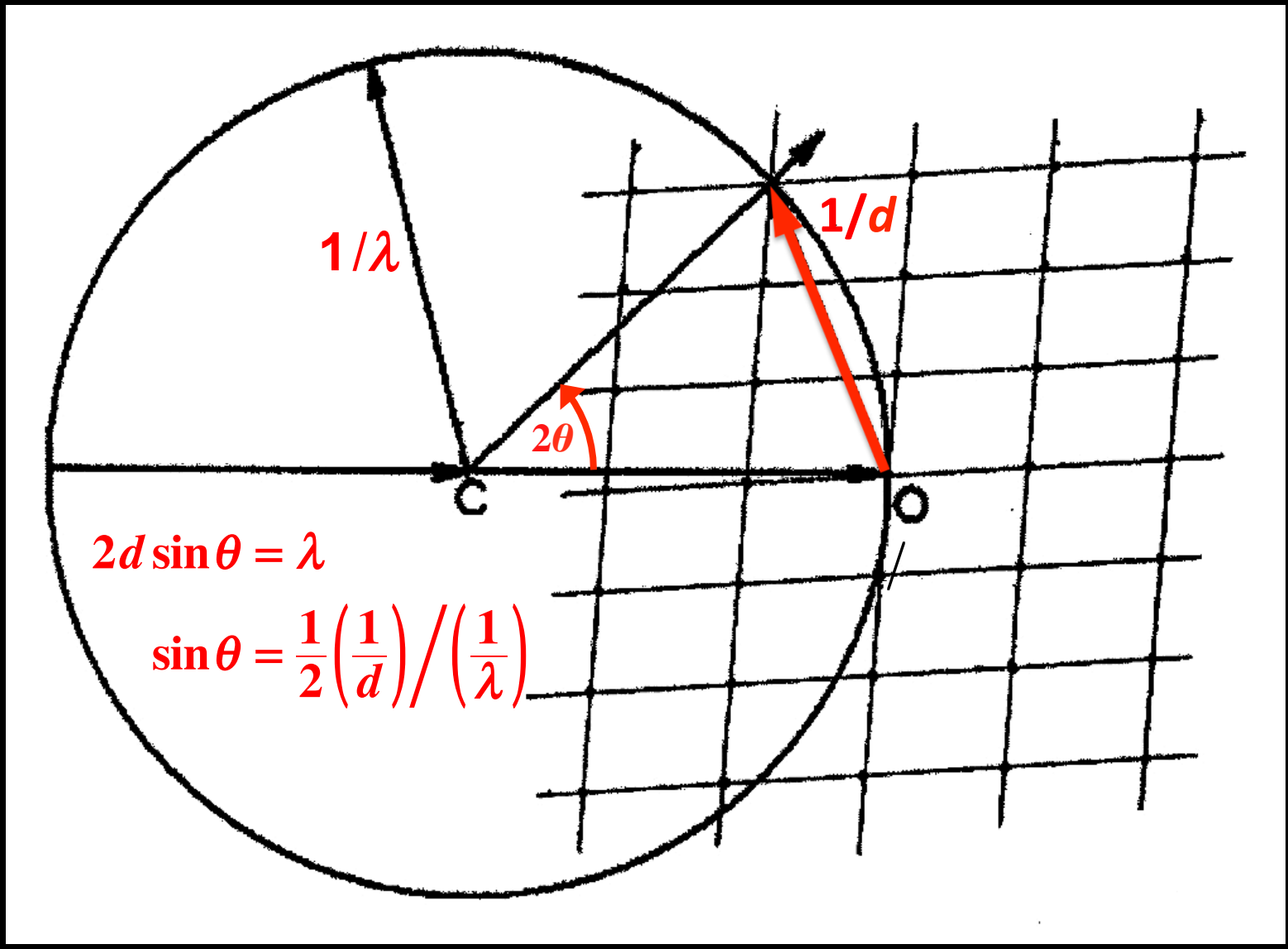


Wm. Henry & Wm. Lawrence Bragg (1913) $2d\sin\theta = \lambda$

Paul Peter Ewald (1913) $\sin\theta = \frac{1}{d}\frac{\lambda}{2} = \left(\frac{1}{d}\right)\Big/\left(\frac{2}{\lambda}\right)$

Leonid V. Azároff (1968). *Elements of X-ray Crystallography*. McGraw-Hill Book Co.

The Ewald construction on the reciprocal lattice



http://mic.ucla.edu/x-ray%20diffraction/tutorials.htm

The Ewald construction on the reciprocal lattice

$$\frac{\hat{\mathbf{s}}_0}{\lambda} + \mathbf{S} = \frac{\hat{\mathbf{s}}}{\lambda}, \qquad \mathbf{S} = \frac{\hat{\mathbf{s}} - \hat{\mathbf{s}}_0}{\lambda}$$

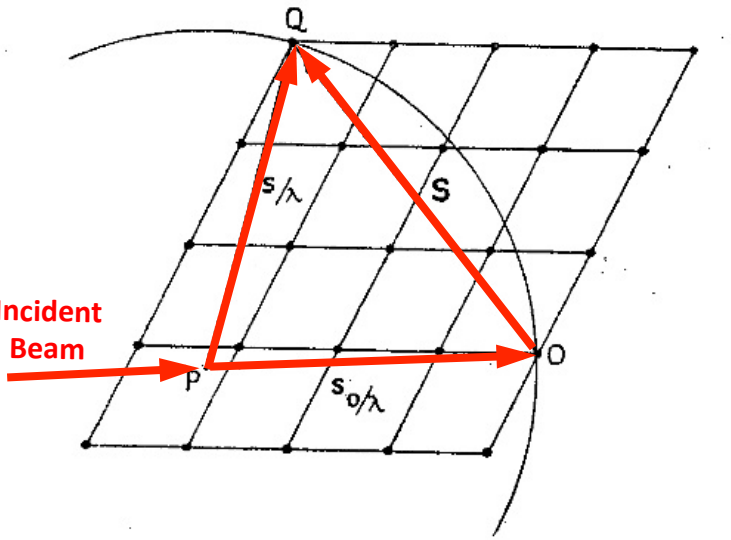


FIG. 3. Ewald's construction for the diffraction maxima, using the reciprocal lattice and the sphere of reflection

$$\measuredangle OPQ = \measuredangle \hat{\mathbf{s}}, \hat{\mathbf{s}}_0 = 2\theta$$

$$\mathbf{S} = \left(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0\right)/\lambda$$

$$|\mathbf{S}| = 2\left(\sin\theta\right)/\lambda = d^*_{hkl} = 1/d_{hkl}$$

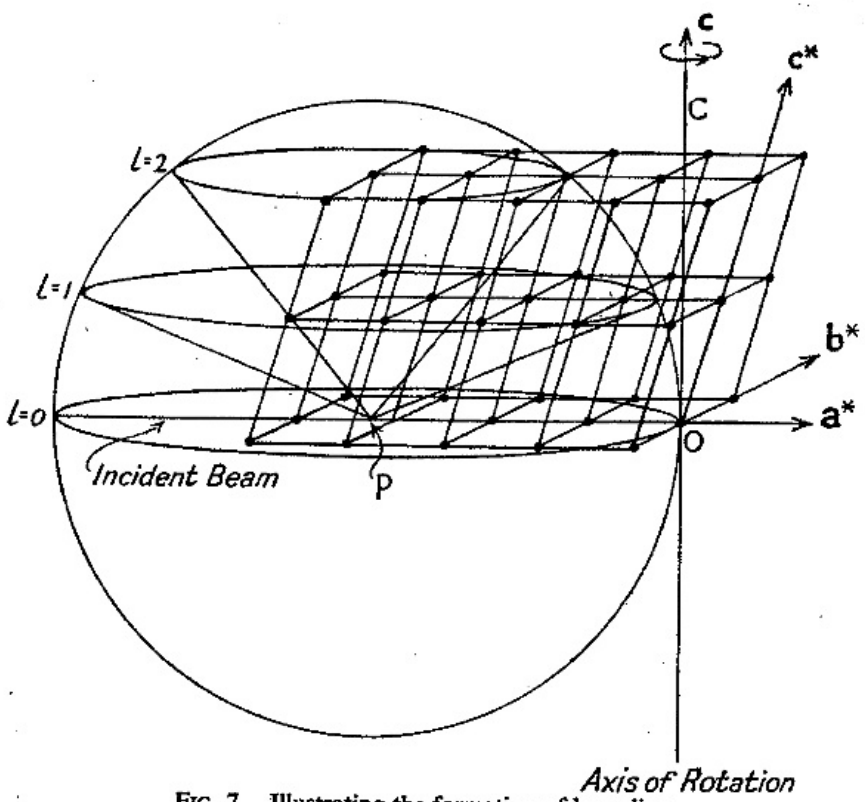


FIG. 7. Illustrating the formation of layer lines

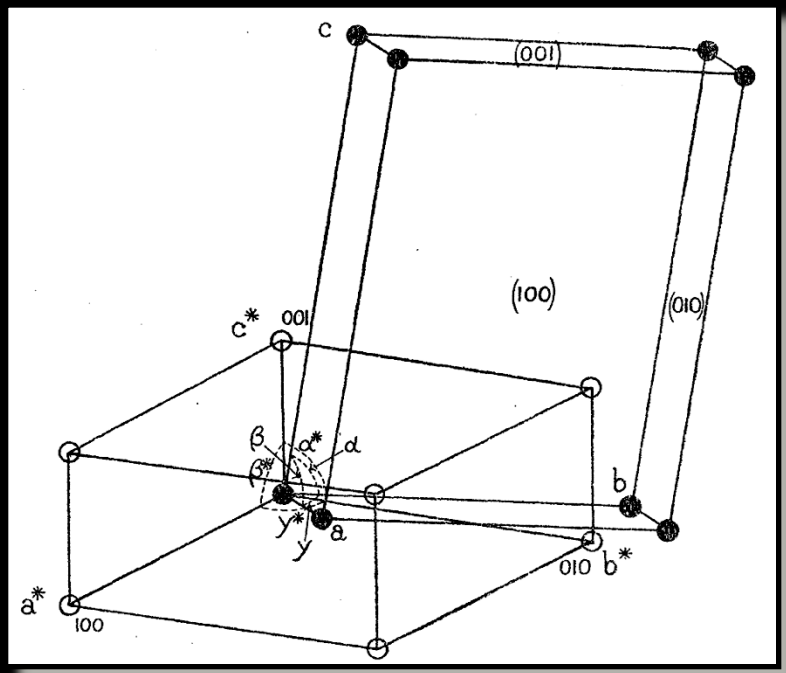
R.W. James (1982). *The Optical Principles of the Diffraction of X-rays*. Woodbridge, Conn.: Ox Bow Press

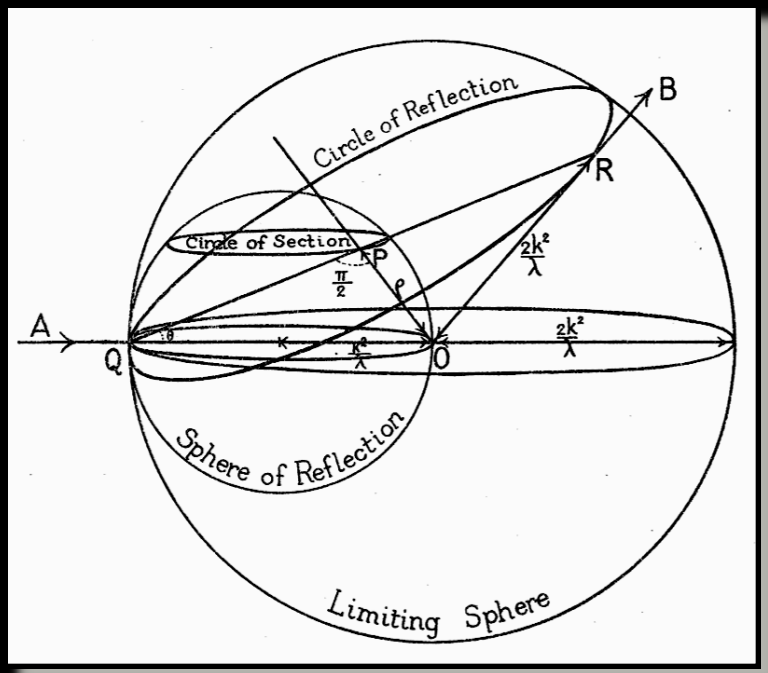
On the Interpretation of X-Ray, Single Crystal, Rotation Photographs.

By J. D. Bernal, B.A.

(Communicated by Sir William Bragg, F.R.S.—Received July 24, 1926.)

In the development of the study of crystals by X-rays the methods used divide themselves naturally into four types: the Bragg Ionisation Spectrometer method, the Laue method, the Powder method of Debye and Scherrer, and the Rotating Crystal method of Rinne, Schiebold and Polyani. The techniques of the first three of these methods are fully explained in such books as 'X-Rays and Crystal Structure,' by W. H. and W. L. Bragg, 'The Structure of Crystals,' by Wyckoff, and 'Krystalle und Rontgenstrahlen,' by Ewald, as well as in original papers. On the other hand, the rotation method is only





Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 113, No. 763. (Nov. 1, 1926), pp. 117-160.

The Ewald sphere along side an Escher sphere

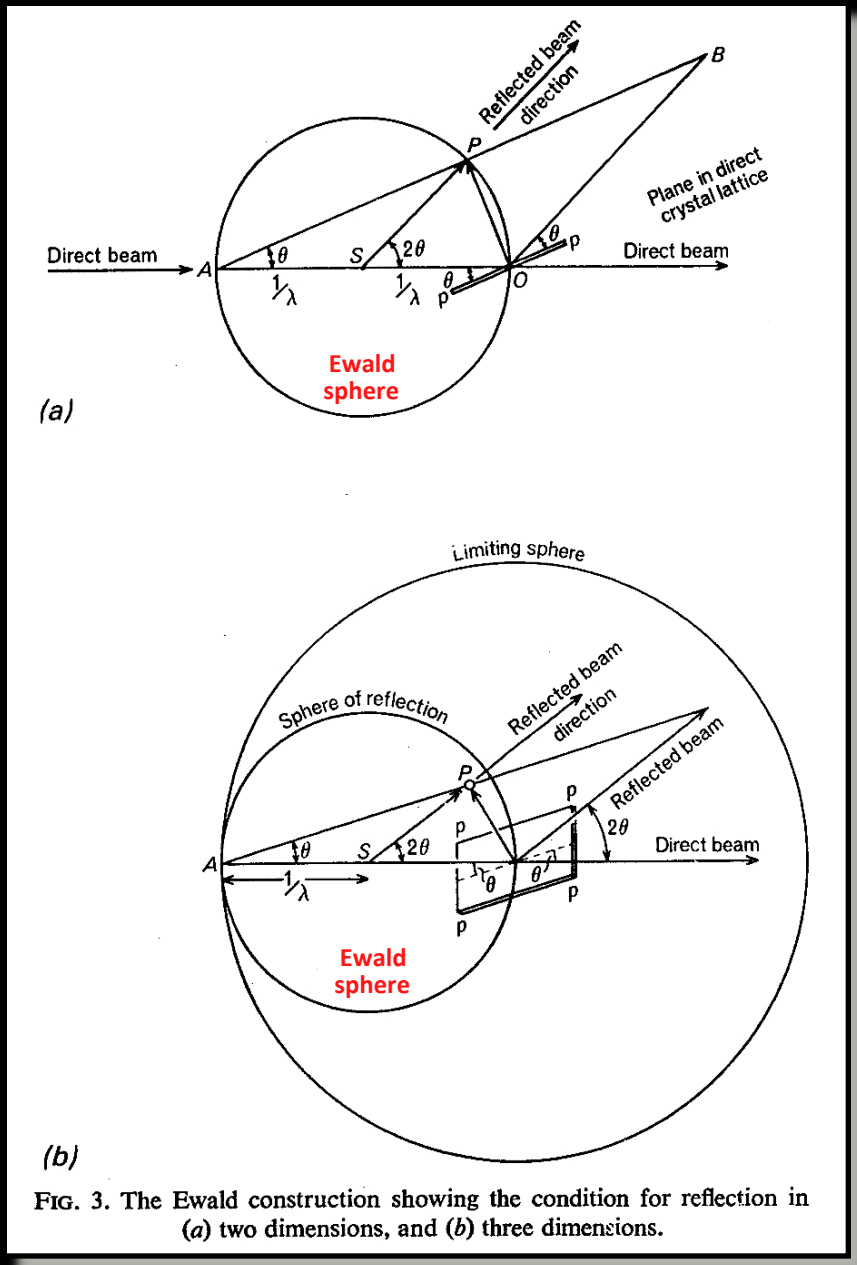
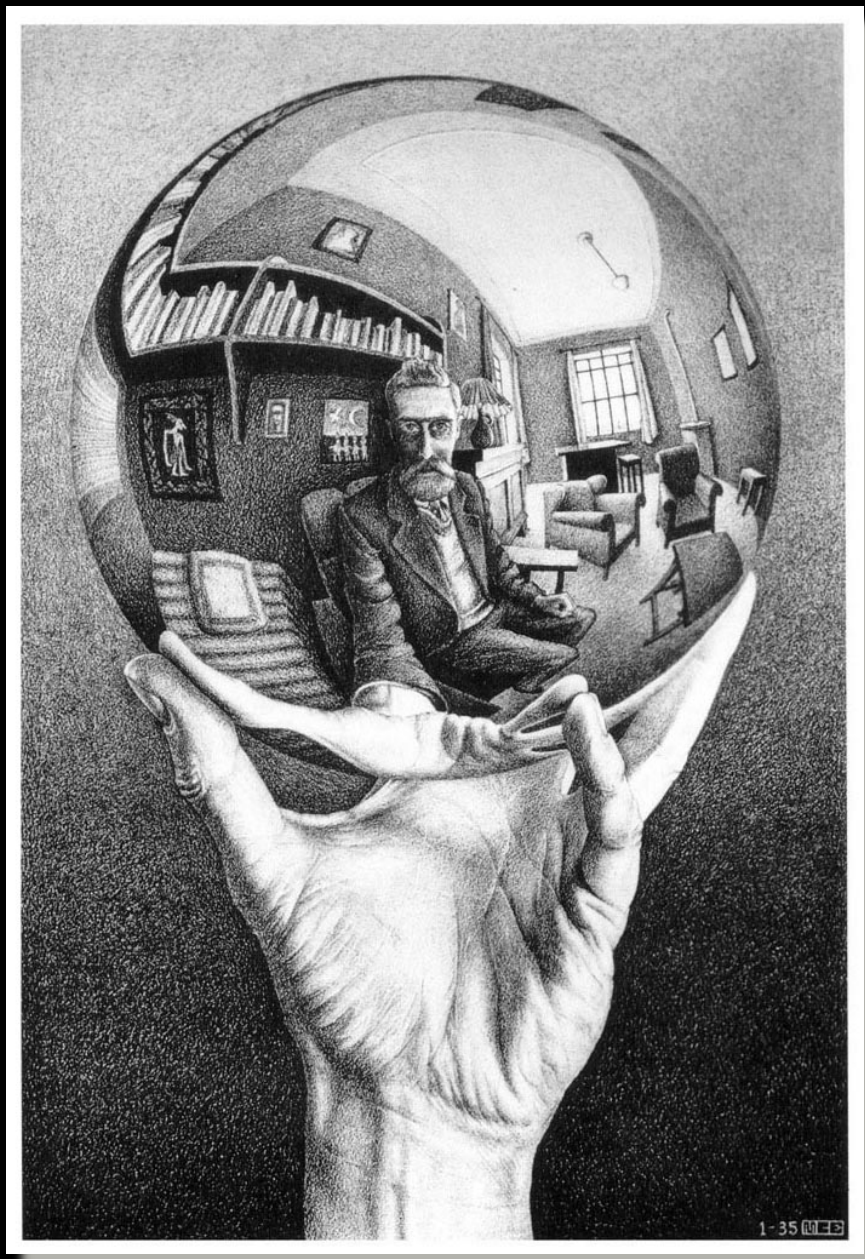


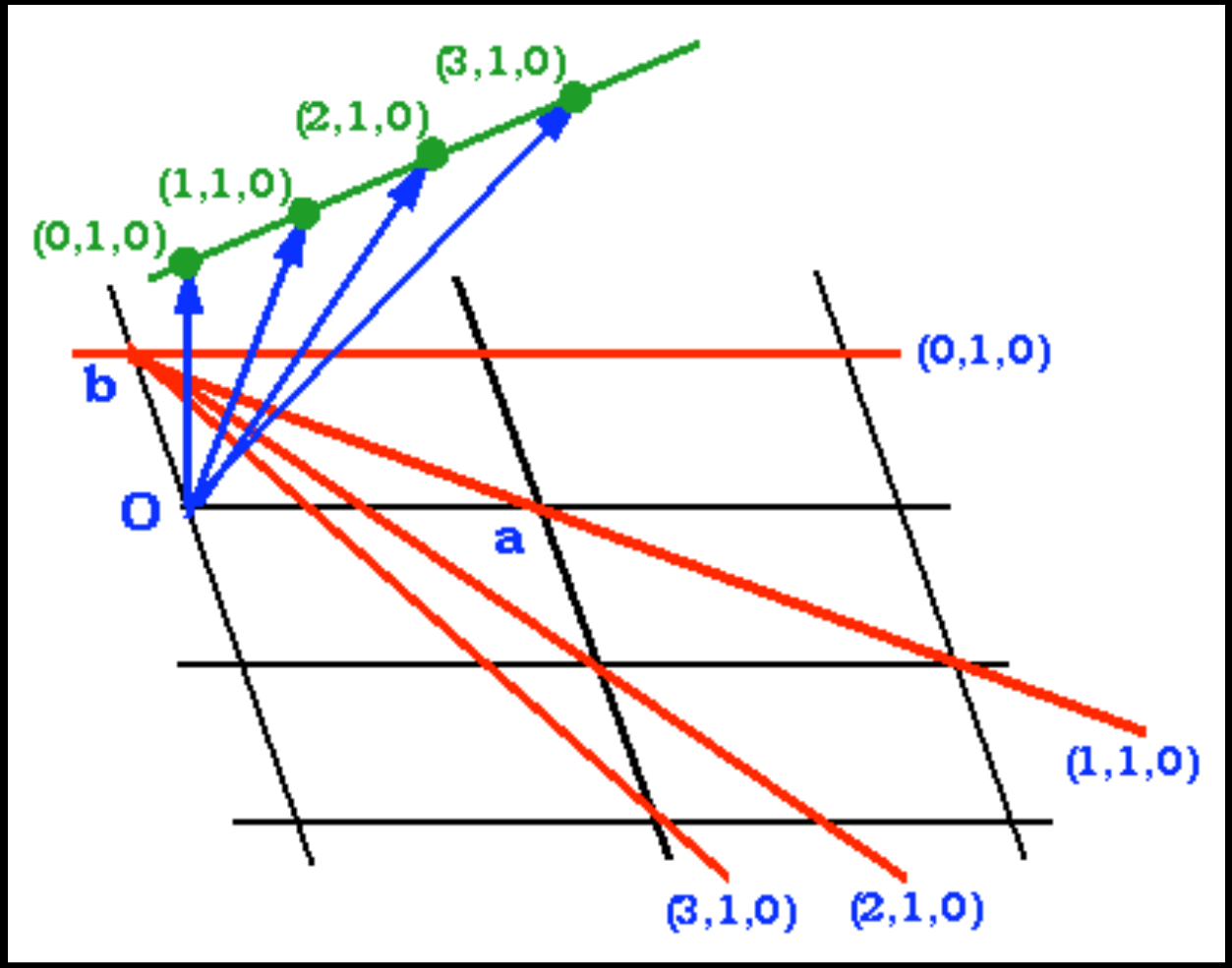
FIG. 3. The Ewald construction showing the condition for reflection in (*a*) two dimensions, and (*b*) three dimensions.



http://www.worldofescher.com/gallery/HandWithSphere.html

Reciprocal lattice points

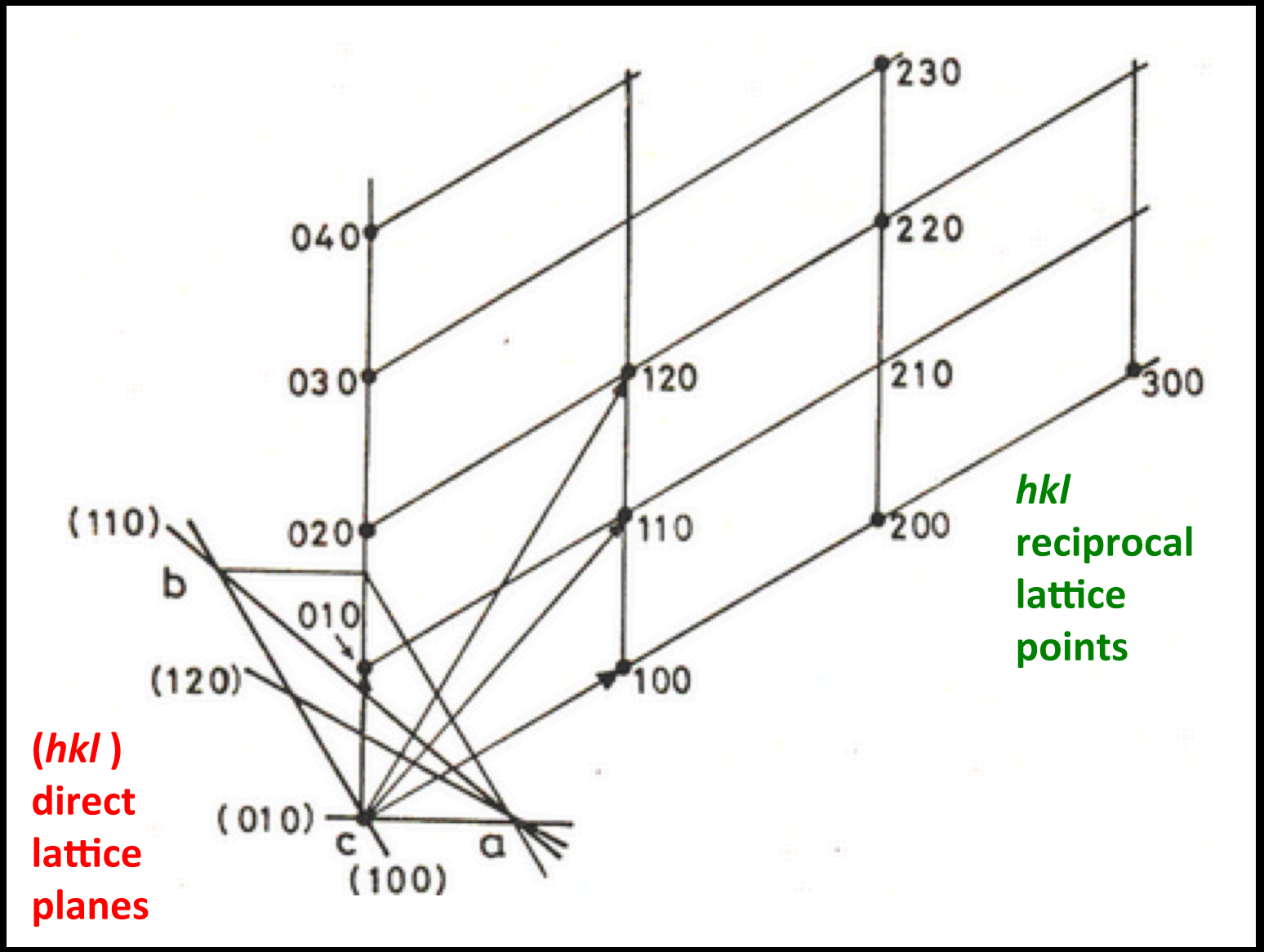
Reciprocal lattice vectors



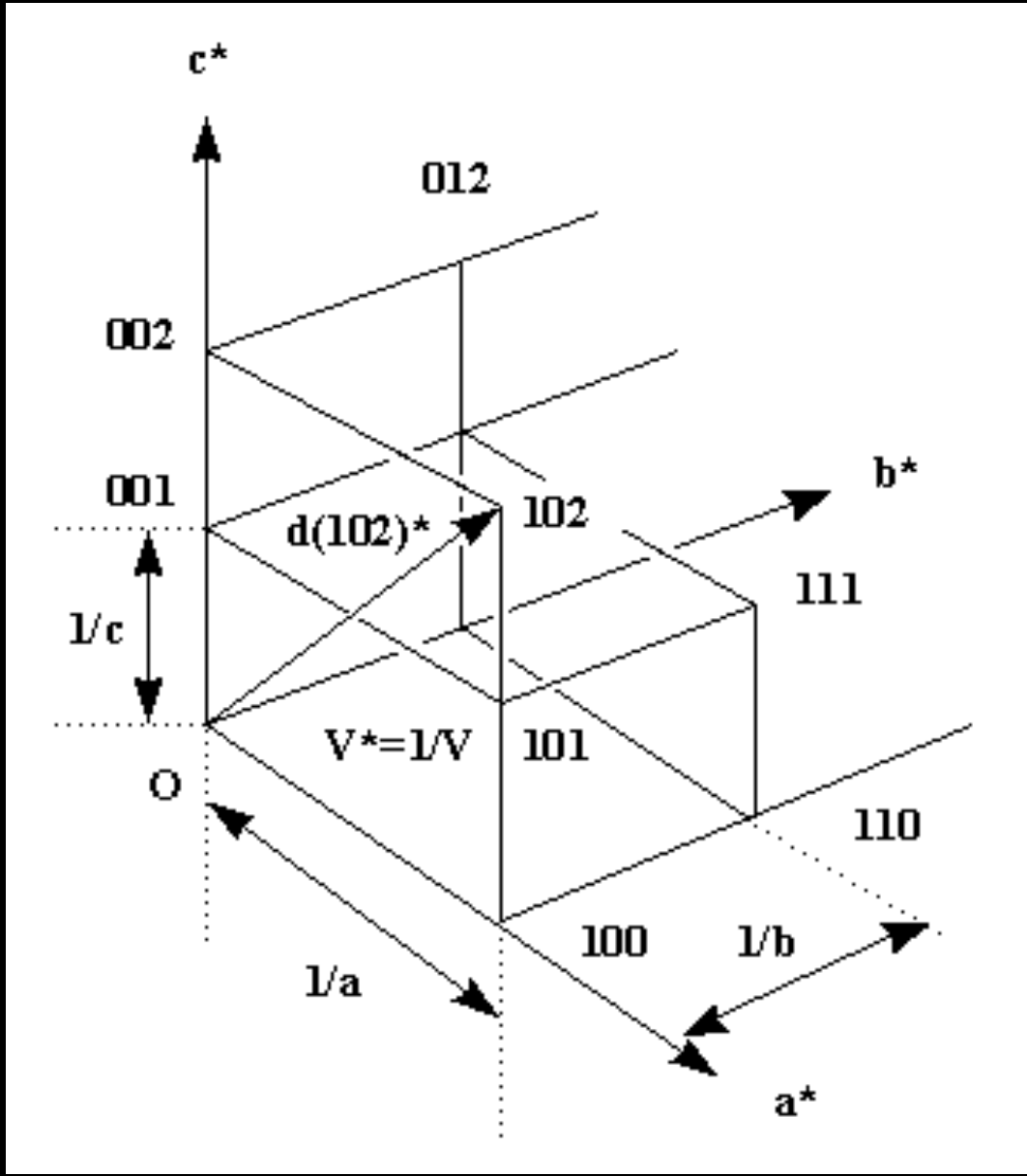
Direct lattice planes

http://www.xtal.igfr.csic.es/Cristalografia/parte_04-en.html

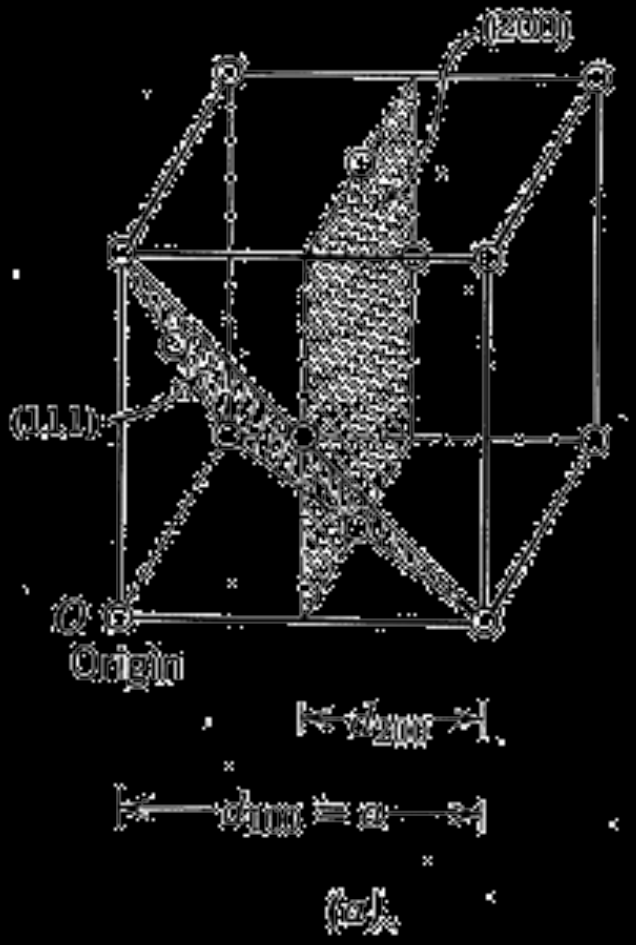
Geometrical construction of a reciprocal lattice

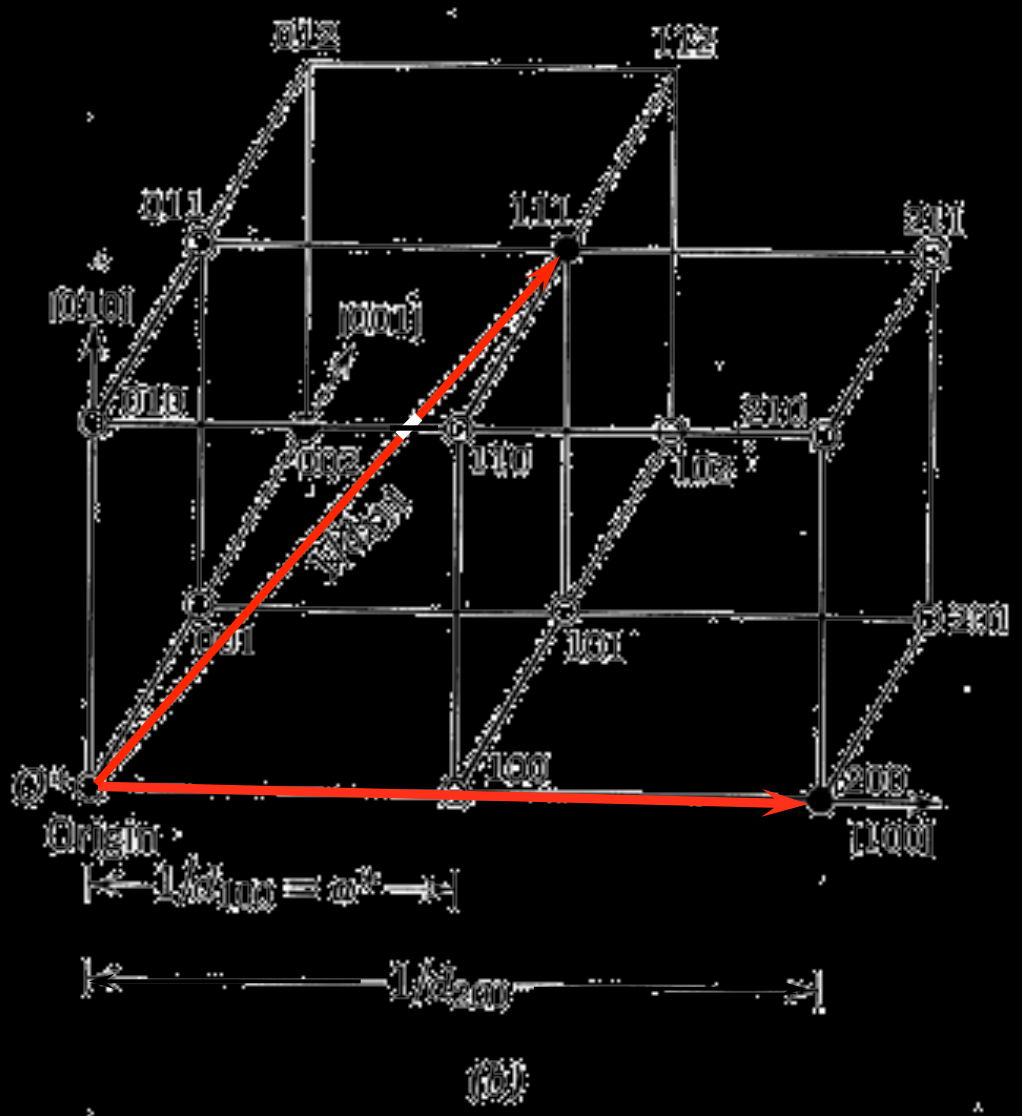


http://ictwiki.iitk.ernet.in/wiki/index.php/Unit-2:_Introduction_to_X-ray_diffraction



http://www.ruppweb.org/Xray/tutorial/spcdiff.htm





http://www.mete.metu.edu.tr/pages/tem/TEMtext/TEMtext.html

a b c Direct Lattice and a* b* c* Reciprocal Lattice

***N.B.* In *all* crystal systems:**

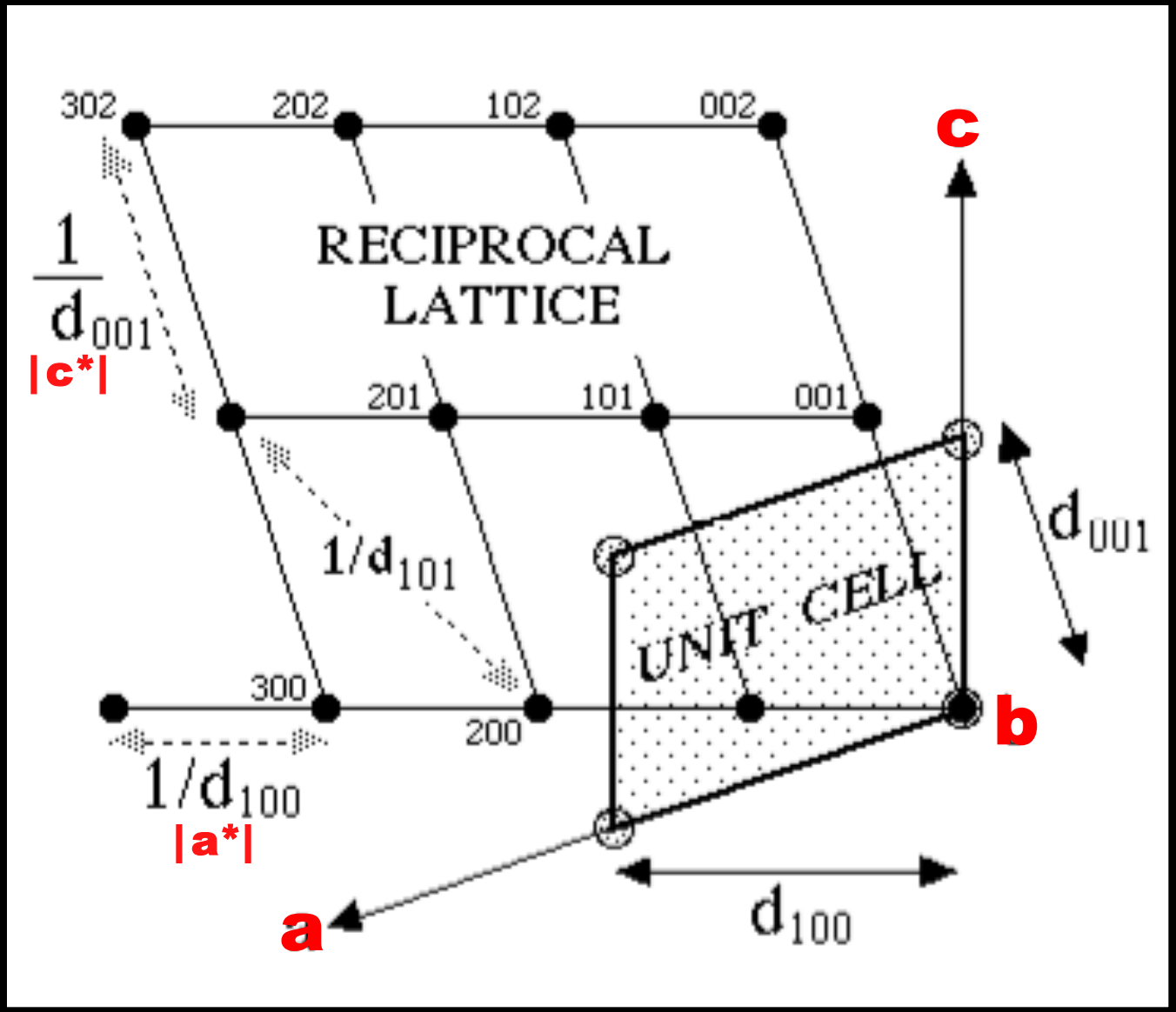
$$\begin{cases} \mathbf{a}^* \perp \mathbf{b} \text{ and } \mathbf{c} \\ \mathbf{b}^* \perp \mathbf{c} \text{ and } \mathbf{a} \\ \mathbf{c}^* \perp \mathbf{a} \text{ and } \mathbf{b} \end{cases}$$

and

$$\begin{cases} \mathbf{a} \perp \mathbf{b}^* \text{ and } \mathbf{c}^* \\ \mathbf{b} \perp \mathbf{c}^* \text{ and } \mathbf{a}^* \\ \mathbf{c} \perp \mathbf{a}^* \text{ and } \mathbf{b}^* \end{cases}$$

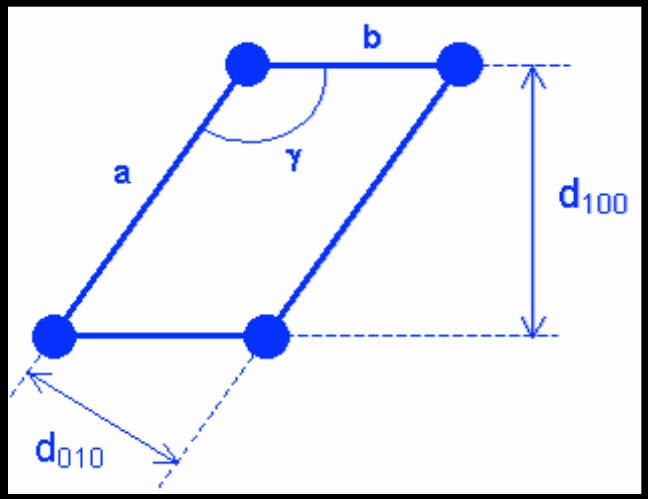
and

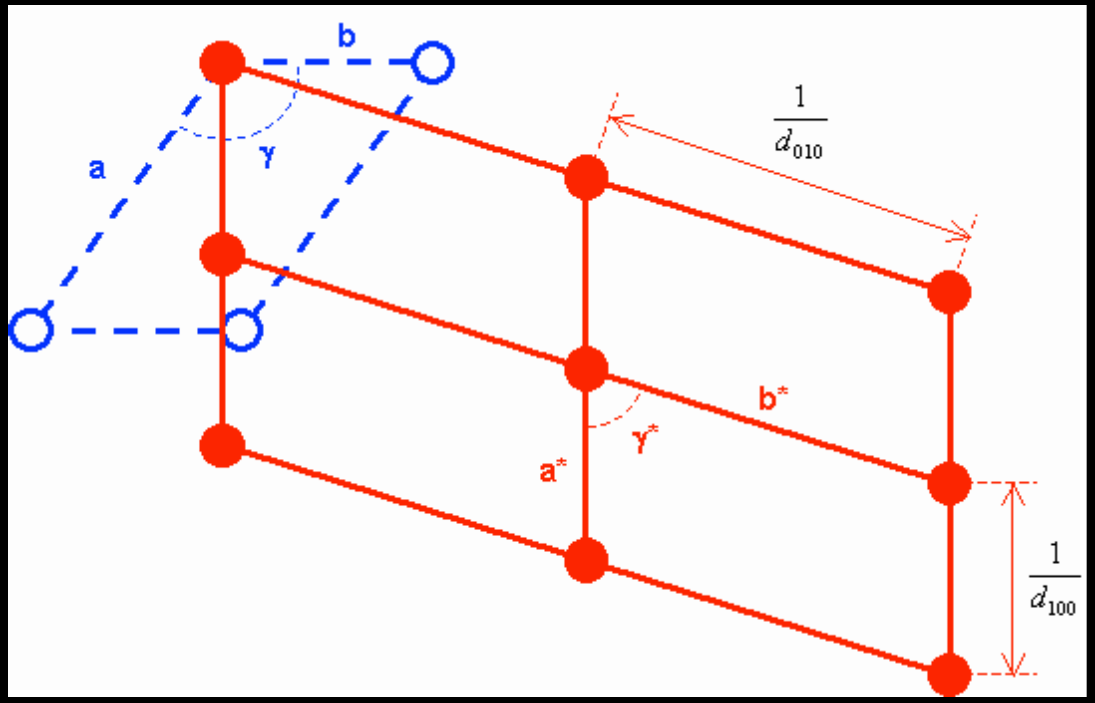
$$\begin{cases} a^* = |\mathbf{a}^*| = 1/d_{100} \\ b^* = |\mathbf{b}^*| = 1/d_{010} \\ c^* = |\mathbf{c}^*| = 1/d_{001} \end{cases}$$



http://www.humboldt.edu/~gdg1/recip.html

Primitive parallelogram lattice



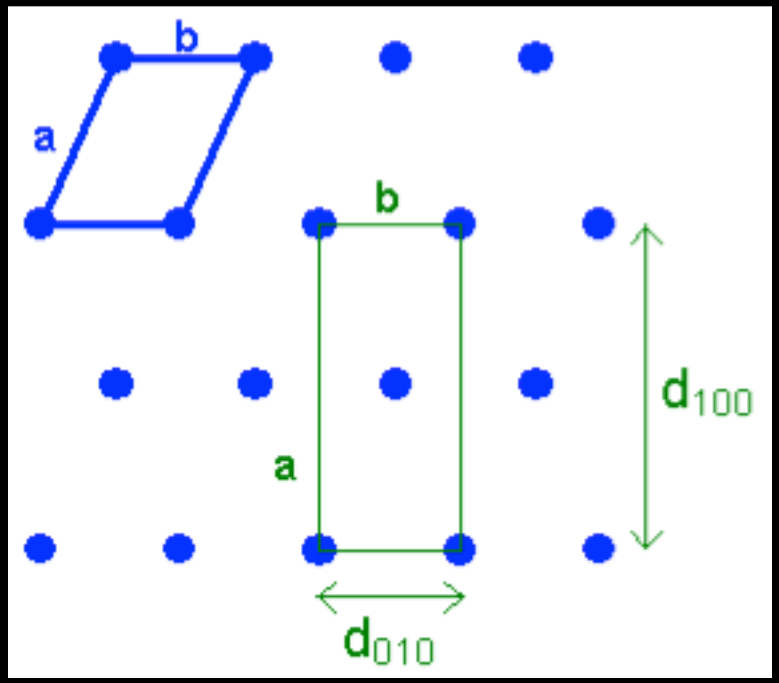


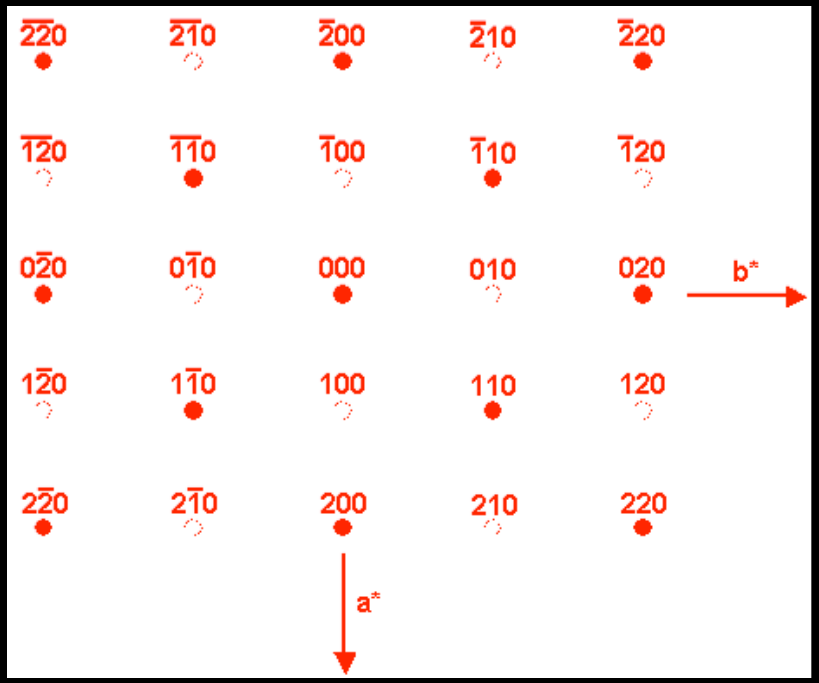
N.B. In *all* crystal systems :

$$\begin{cases} \mathbf{a}^* \perp \mathbf{b} \text{ and } \mathbf{c} \\ \mathbf{b}^* \perp \mathbf{c} \text{ and } \mathbf{a} \\ \mathbf{c}^* \perp \mathbf{a} \text{ and } \mathbf{b} \end{cases} \textit{and} \begin{cases} \mathbf{a} \perp \mathbf{b}^* \text{ and } \mathbf{c}^* \\ \mathbf{b} \perp \mathbf{c}^* \text{ and } \mathbf{a}^* \\ \mathbf{c} \perp \mathbf{a}^* \text{ and } \mathbf{b}^* \end{cases} \textit{and} \begin{cases} a^* = |\mathbf{a}^*| = 1/d_{100} \\ b^* = |\mathbf{b}^*| = 1/d_{010} \\ c^* = |\mathbf{c}^*| = 1/d_{001} \end{cases}$$

http://www.doitpoms.ac.uk/tlplib/xray-diffraction/reciprocal1.php

Centered rectangular lattice





N.B. In *all* crystal systems :

$$\begin{cases} \mathbf{a}^* \perp \mathbf{b} \text{ and } \mathbf{c} \\ \mathbf{b}^* \perp \mathbf{c} \text{ and } \mathbf{a} \\ \mathbf{c}^* \perp \mathbf{a} \text{ and } \mathbf{b} \end{cases} \quad \textbf{\textit{and}} \quad \begin{cases} \mathbf{a} \perp \mathbf{b}^* \text{ and } \mathbf{c}^* \\ \mathbf{b} \perp \mathbf{c}^* \text{ and } \mathbf{a}^* \\ \mathbf{c} \perp \mathbf{a}^* \text{ and } \mathbf{b}^* \end{cases} \quad \textbf{\textit{and}} \quad \begin{cases} a^* = |\mathbf{a}^*| = 1/d_{100} \\ b^* = |\mathbf{b}^*| = 1/d_{010} \\ c^* = |\mathbf{c}^*| = 1/d_{001} \end{cases}$$

http://www.doitpoms.ac.uk/tlplib/xray-diffraction/reciprocal1.php

A family of lattice planes in real space
corresponds to
a point in reciprocal space.

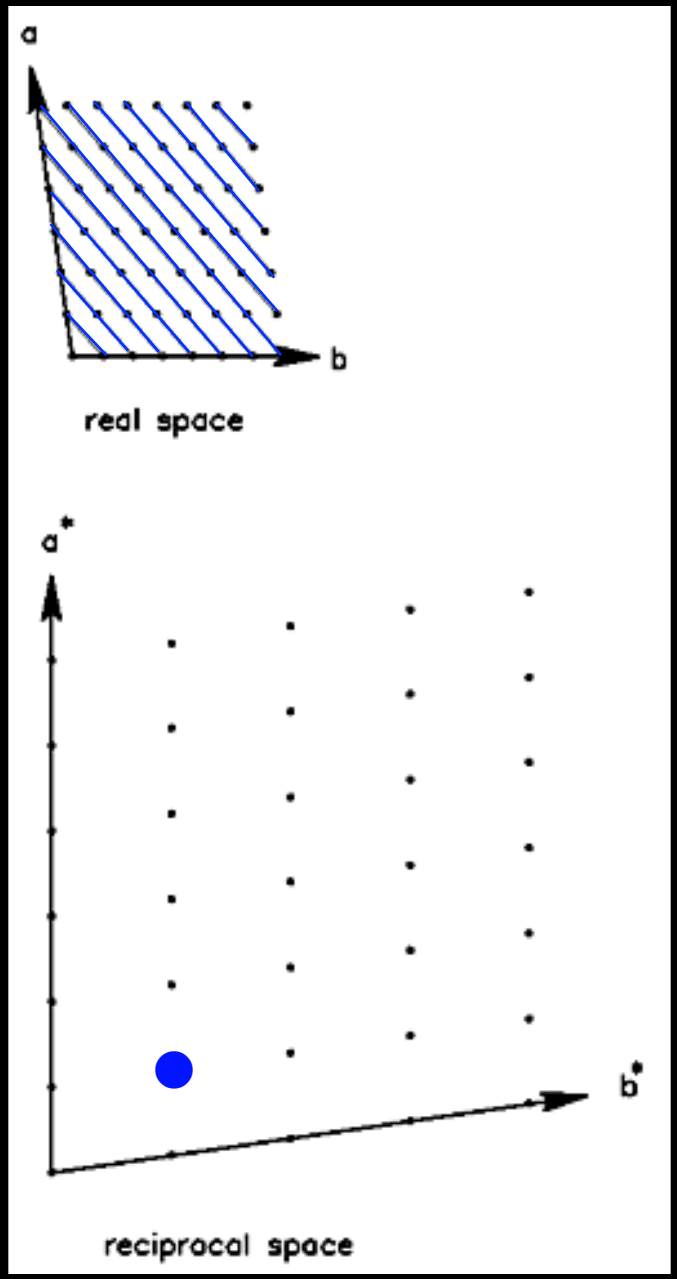
110 lattice planes

N.B. **In *all* crystal systems:**

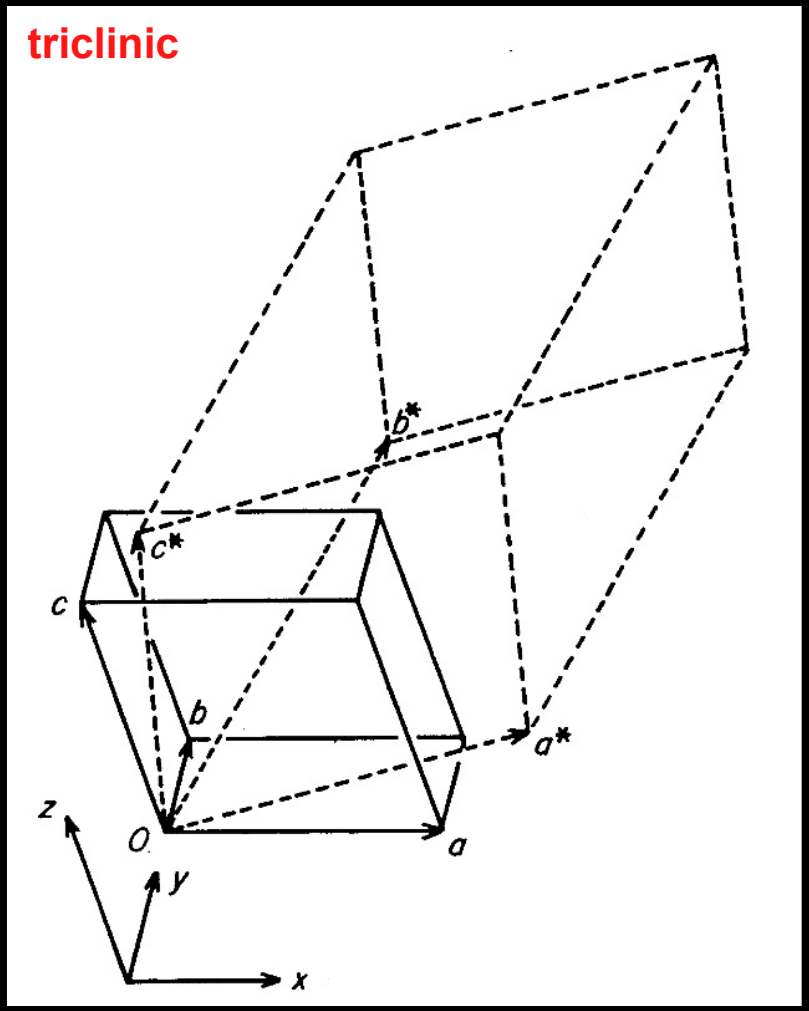
$$\begin{cases} \mathbf{a}^* \perp \mathbf{b} \text{ and } \mathbf{c} \\ \mathbf{b}^* \perp \mathbf{c} \text{ and } \mathbf{a} \\ \mathbf{c}^* \perp \mathbf{a} \text{ and } \mathbf{b} \end{cases} \quad \textbf{and} \quad \begin{cases} \mathbf{a} \perp \mathbf{b}^* \text{ and } \mathbf{c}^* \\ \mathbf{b} \perp \mathbf{c}^* \text{ and } \mathbf{a}^* \\ \mathbf{c} \perp \mathbf{a}^* \text{ and } \mathbf{b}^* \end{cases}$$

$$\textbf{and} \quad \begin{cases} a^* = |\mathbf{a}^*| = 1/d_{100} \\ b^* = |\mathbf{b}^*| = 1/d_{010} \\ c^* = |\mathbf{c}^*| = 1/d_{001} \end{cases}$$

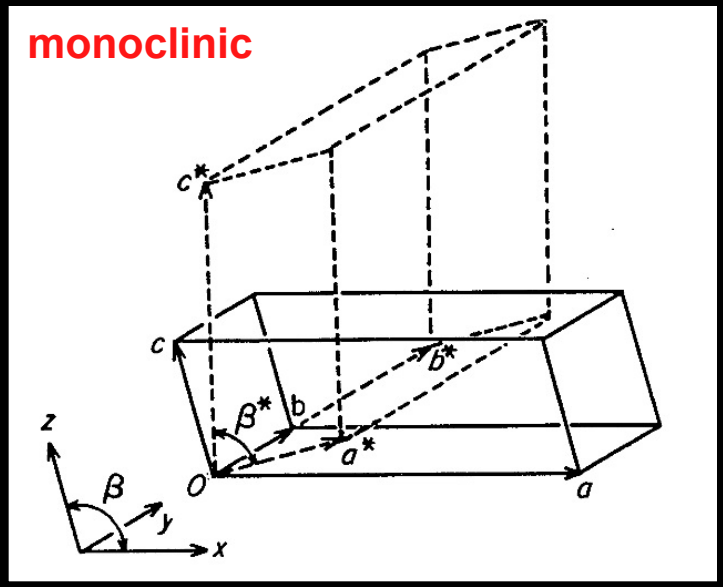
110 reciprocal lattice point



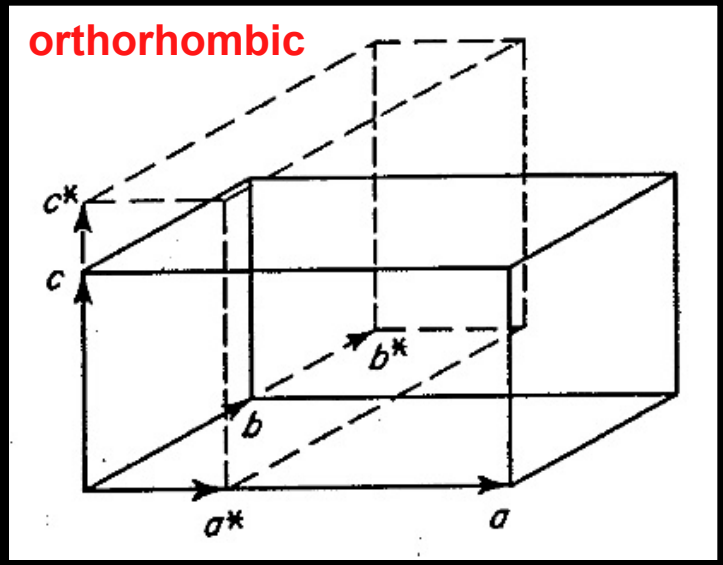
triclinic



monoclinic

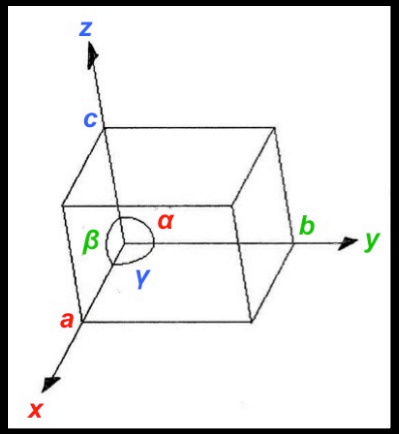


orthorhombic



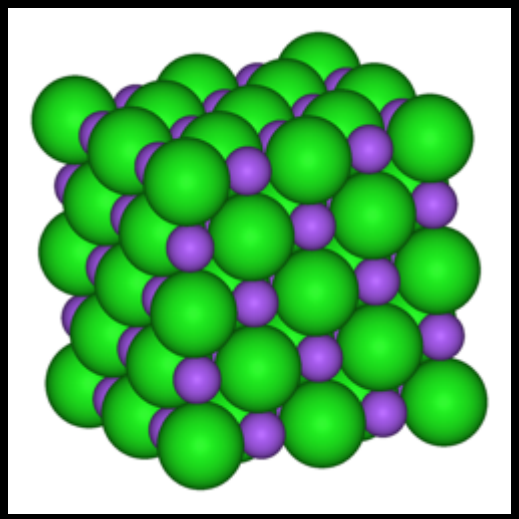
N.B. **In *all* crystal systems:**

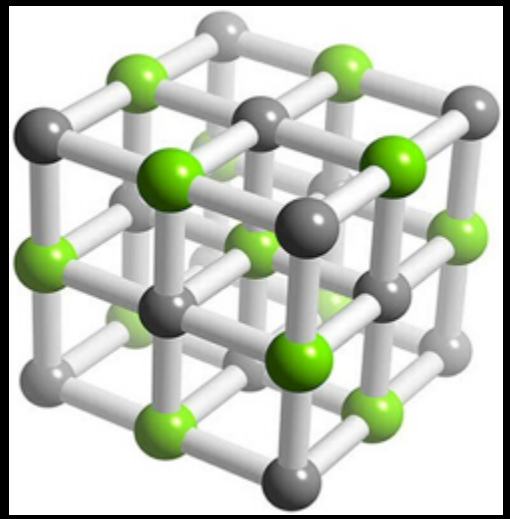
$$\begin{cases} \mathbf{a}^* \perp \mathbf{b} \text{ and } \mathbf{c} \\ \mathbf{b}^* \perp \mathbf{c} \text{ and } \mathbf{a} \\ \mathbf{c}^* \perp \mathbf{a} \text{ and } \mathbf{b} \end{cases} \quad \textbf{\textit{and}} \quad \begin{cases} \mathbf{a} \perp \mathbf{b}^* \text{ and } \mathbf{c}^* \\ \mathbf{b} \perp \mathbf{c}^* \text{ and } \mathbf{a}^* \\ \mathbf{c} \perp \mathbf{a}^* \text{ and } \mathbf{b}^* \end{cases} \quad \textbf{\textit{and}} \quad \begin{cases} a^* = |\mathbf{a}^*| = 1/d_{100} \\ b^* = |\mathbf{b}^*| = 1/d_{010} \\ c^* = |\mathbf{c}^*| = 1/d_{001} \end{cases}$$


z
c
α
β
γ
b
y
a
x

The Braggs' first crystal structures (1913)

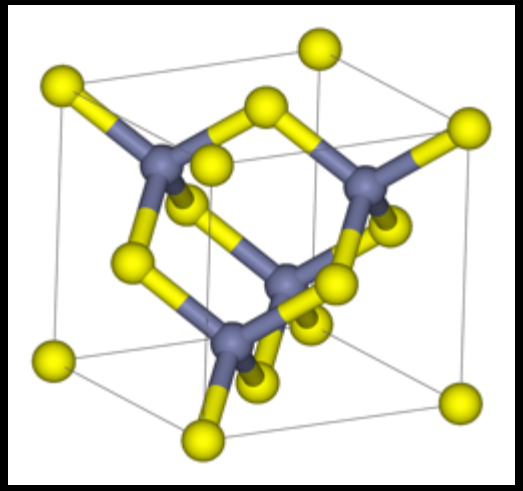
NaCl
rock salt
halite

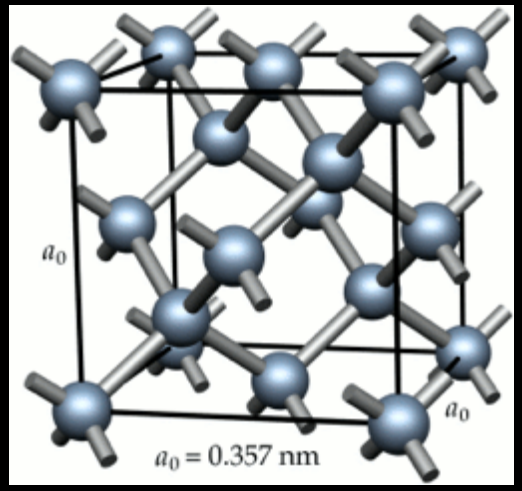




KCl
sylvite

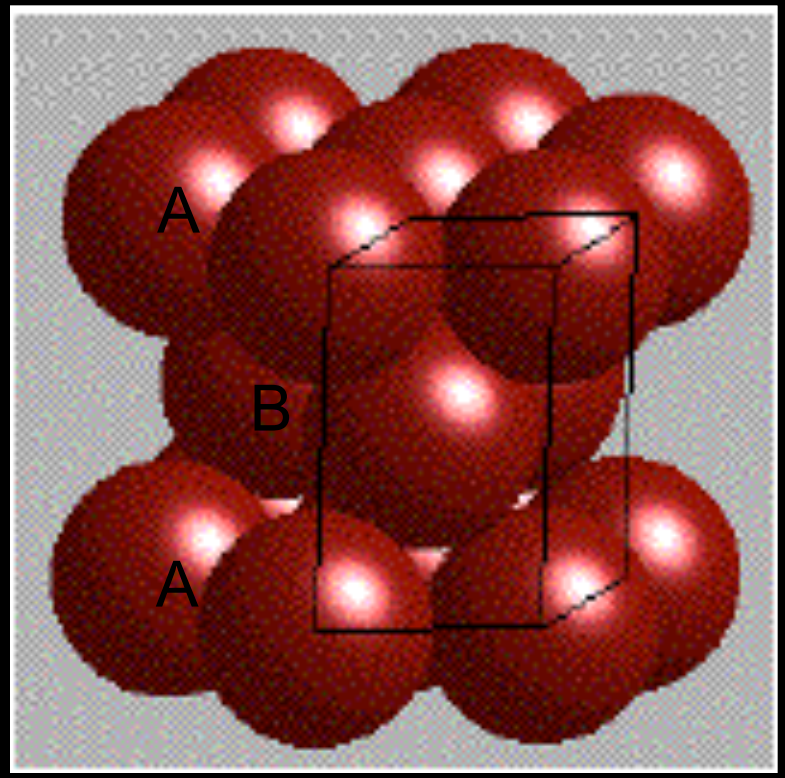
ZnS
zinc blende
spahlerite

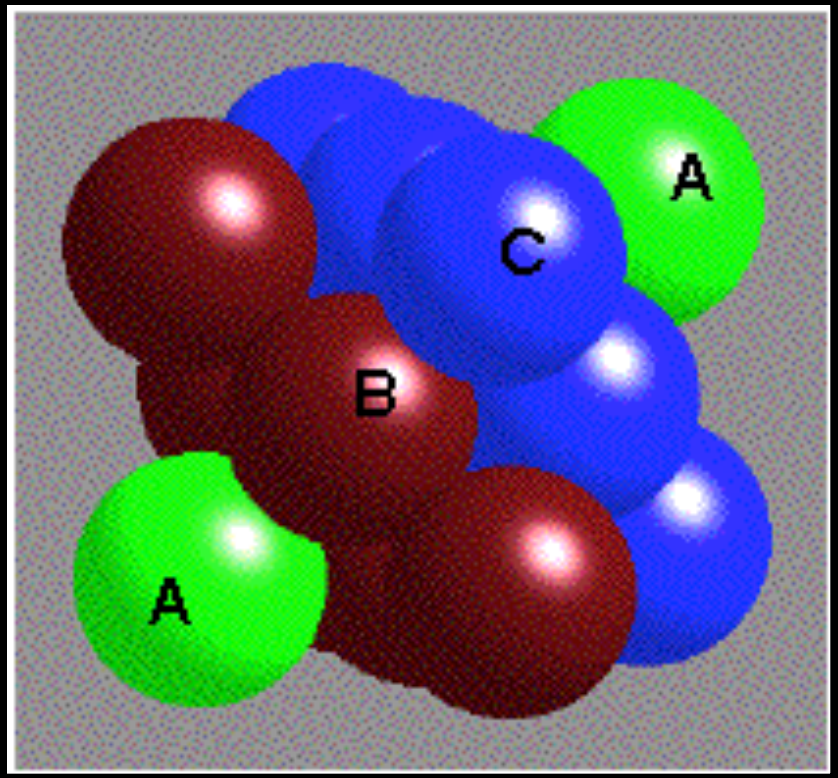




http://newton.ex.ac.uk/research/qsystems/people/sque/diamond/structure/structure.html

Closest packing of spheres (Kepler's conjecture, 1611)



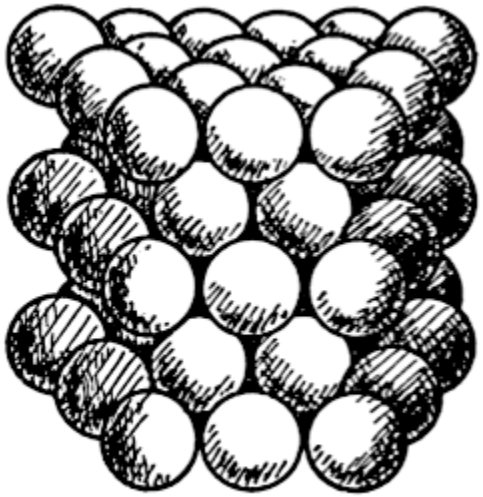


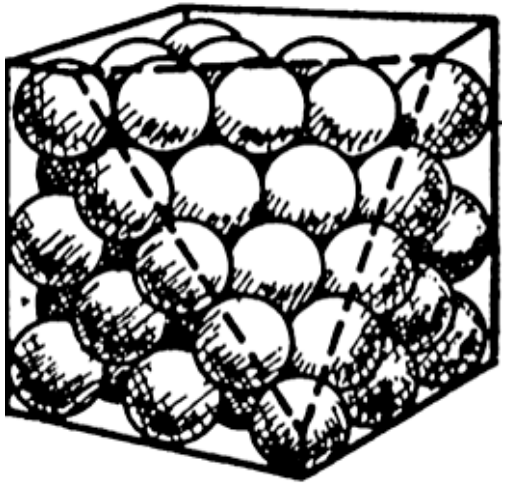
HCP
ABA…

CCP = FCC
ABCA

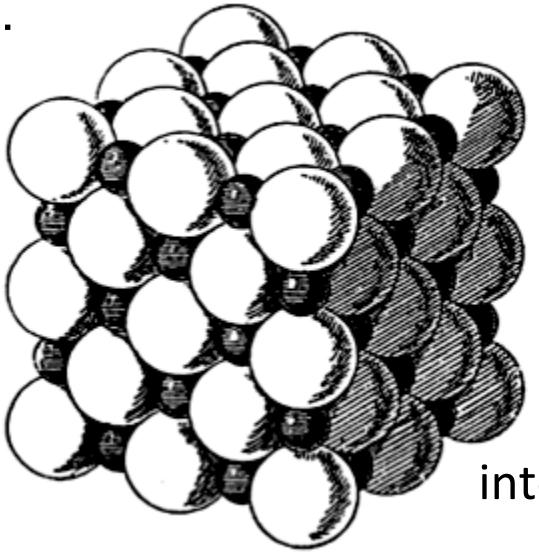
http://www.ncl.ox.ac.uk/icl/heyes/structure_of_solids/Lecture1/Lec1.html

William Barlow (1898) and William Jackson Pope (1906)



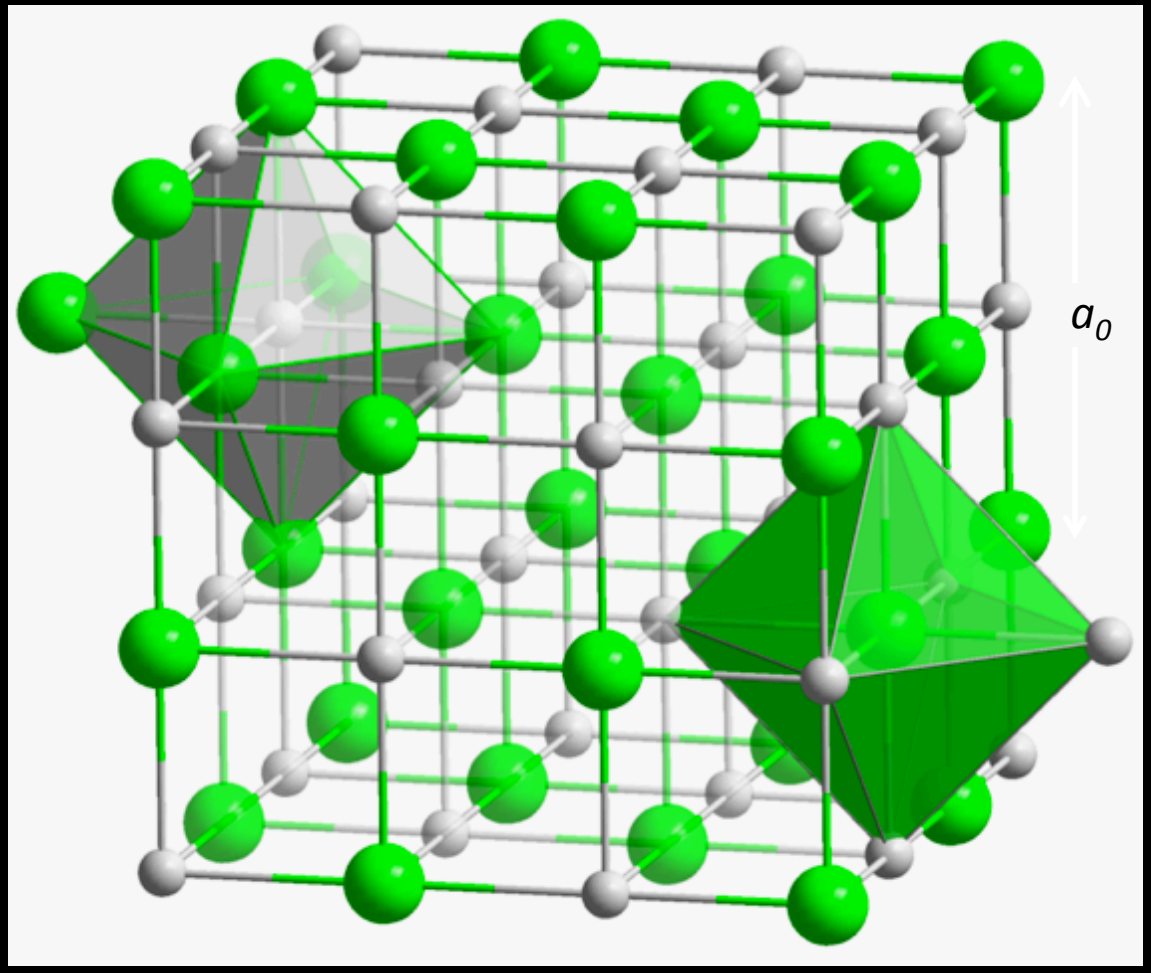


hcp
ABA…



NaCl
interpenetrating
fcc

Hypothetical crystal structures based on sphere-packing



$$\sin\theta_{hkl} = \frac{n\lambda}{2d_{hkl}}$$

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

$$d_{100} = a_0$$

$$d_{110} = a_0/\sqrt{2} = 0.707\,a_0$$

$$d_{111} = a_0/\sqrt{3} = 0.577\,a_0$$

$$d_{200} = a_0/2$$

$$d_{210} = a_0/\sqrt{5} = 0.447\,a_0$$

$$d_{211} = a_0/\sqrt{6} = 0.408\,a_0$$

$$\vdots$$

$$a_0 = \sqrt[3]{V_{\text{cell}}} = \sqrt[3]{\frac{Z_{\text{cell}}\,M_{\text{r}}}{\rho_{\text{m}}\,N_{\text{A}}}}$$

$$= \sqrt[3]{\frac{4 \times 58.5 \times 10^{24}\ \text{Å}^3}{2.16 \times 6.02 \times 10^{23}}} = 5.63\text{Å}$$

NaCl formula unit, $\text{Na}^+\left(\text{Cl}^-\right)_{6\times\frac{1}{6}}$, $\text{Cl}^-\left(\text{Na}^+\right)_{6\times\frac{1}{6}}$, $M_{\text{r}} = 23.0 + 35.5 = 58.5$ Da

Interpenetrating face-centered cubic unit cell, $Z_{\text{cell}} = 4\text{NaCl}$

$$\underbrace{\left(8\times\tfrac{1}{8}\right)}_{\text{corner Na}^+} + \underbrace{\left(6\times\tfrac{1}{2}\right)}_{\text{face Na}^+} = 1+3 = 4 \begin{cases} \text{Na}^+ \\ \text{Cl}^- \end{cases} \quad \text{and} \quad \underbrace{\left(12\times\tfrac{1}{4}\right)}_{\text{edge Cl}^-} + \underbrace{1}_{\substack{\text{center} \\ \text{Cl}^-}} = 3+1 = 4 \begin{cases} \text{Cl}^- \\ \text{Na}^+ \end{cases}$$