3.012 Fund of Mat Sci: Structure – Lecture 17

X-RAY DIFFRACTION

Image of a spiral sea shell (left) and Rosalyn Franklin's original picture of a DNA Alpha Helix (right).
Images removed for copyright reasons.

A beautiful spiral, and …   an even more beautiful one

Homework for Wed Nov 9

- Read: Prof Wuensch Lecture Notes

① QUIZ 2 : VARIATIONAL PRINCIPLE

8 1/2 → 15

② ISS & ASHLEY : THU 7-9pm

③ OFFICE HOURS :

④ WULFF LECTURE 3.30pm 10-250

PROF. THOMAS

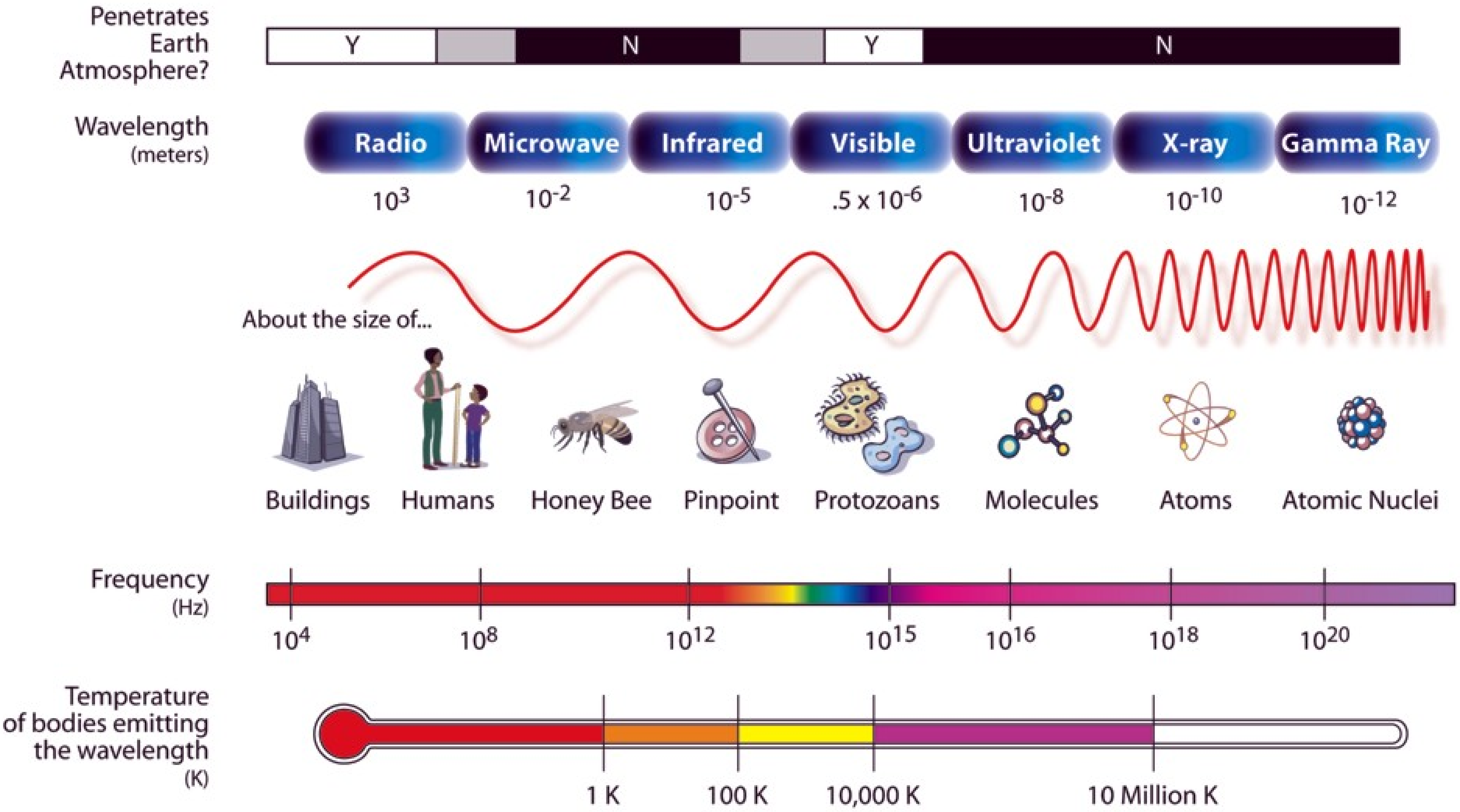
Last time:

1. Glide planes, screw axes
2. Space groups
3. Bravais lattices: sc, bcc, fcc (also, lattice with a basis)
4. Primitive, conventional, and Wigner-Seitz cells
5. Miller indices
6. Diamond, zincblend, perovskites, rocksalt, CsCl

Probing with radiation

- Wavelength need to be smaller than typical interatomic distances
- Beams of photon (X-rays), electrons, neutrons
- We look at coherent (all same atoms behave in the same way), elastic (no energy is lost) scattering
- Elastic: diffraction. Inelastic: spectroscopies
- We “interrogate” long-range order with coherent elastic scattering

THE ELECTROMAGNETIC SPECTRUM



Examples: http://imagers.gsfc.nasa.gov/ems/ems.html

Energy of an accelerated electron

$$\Delta E = eV = h\upsilon = \frac{hc}{\lambda}$$

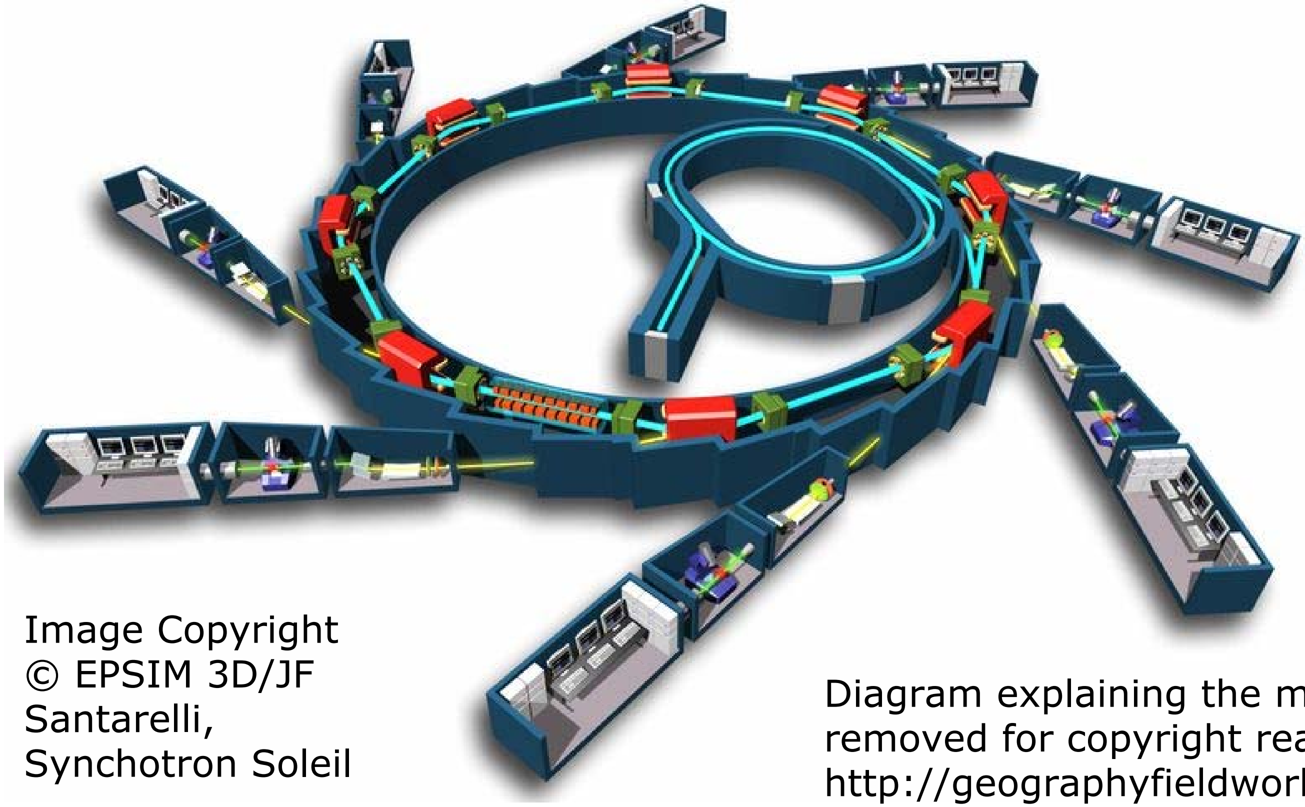
$$V = \frac{\left(6.626\times10^{-34}\ J-\sec\right)\left(2.998\times10^{10}\ {}^{cm}\!/_{\sec}\right)}{\left(10^{-8}\ {}^{cm}\!/_{\text{Å}}\right)\left(1.602\times10^{-19}\ {}^{J}\!/_{V}\right)}$$

$$= 12.4\times10^{3}\ {}^{V}\!/_{\text{Å}}$$

$$kV = {}^{12.4}\!/_{\lambda} \qquad \lambda[=]\text{Å}$$

How do we generate soft X-rays (~1000 eV)?

- Relativistic effects: every time a charge is accelerated or decelerated: wigglers and undulators in a synchrotron



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Santarelli,
Synchotron Soleil

Diagram explaining the mechanics of a synchrotron removed for copyright reasons. See http://geographyfieldwork.com/SynchrotronWorks.htm

How do we generate soft X-rays?

- In the lab: beam of electrons striking a metal target
  - Electrons are decelerated, and they emit radiation on a broad spectrum of frequencies. This is called *Bremmstrahlung*
  - In addition, we excite core electrons, that decay back emitting radiation at K, L, M lines

Moseley law

$$h\upsilon_{L\alpha} = 13.6\text{eV}\ \ (Z - 7.4)^2 \left[\frac{1}{2^2} - \frac{1}{3^2}\right]$$

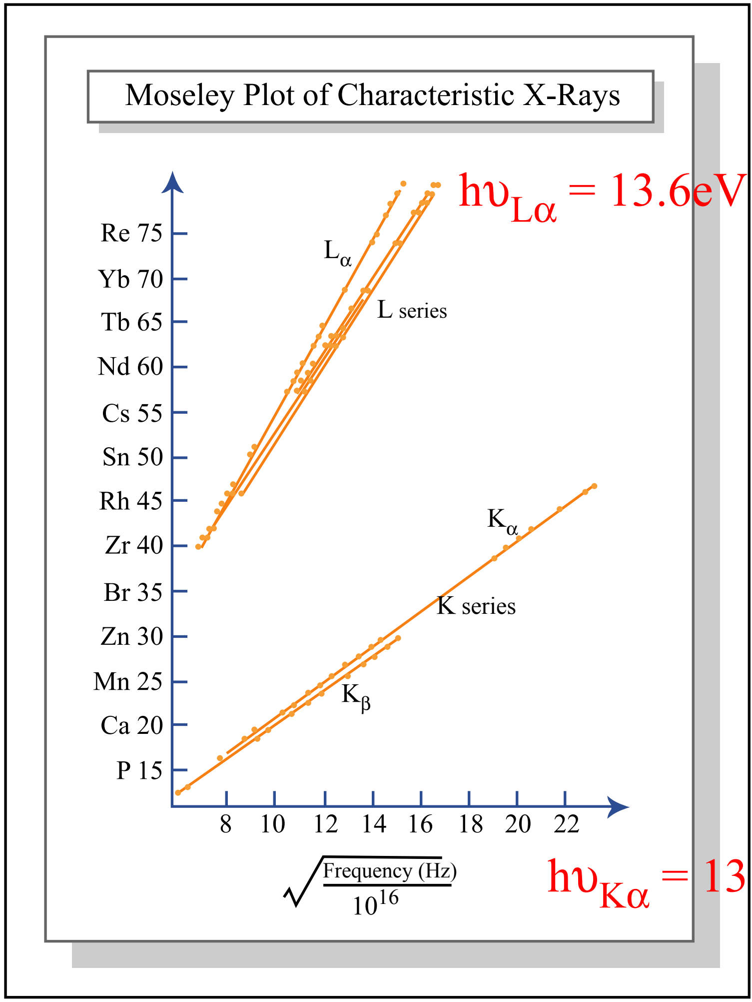


Figure by MIT OCW.

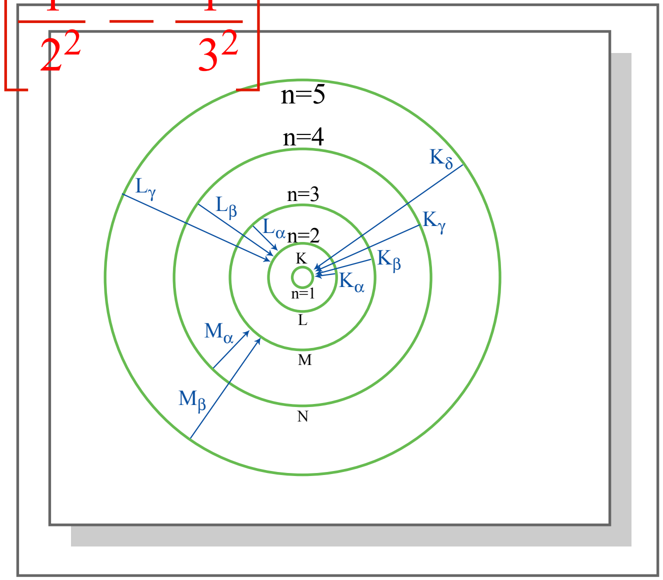
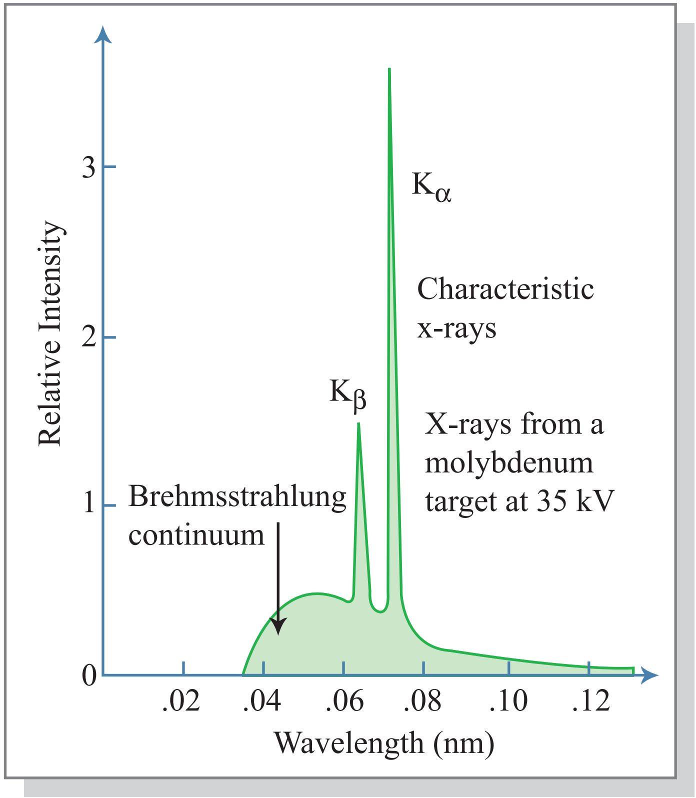


Figure by MIT OCW.

$$h\upsilon_{K\alpha} = 13.6\text{eV}\ \ (Z - 1)^2 \left[\frac{1}{1^2} - \frac{1}{2^2}\right] = \frac{3}{4} 13.6\ (Z - 1)^2\ \text{eV}$$

How do we generate X-rays?



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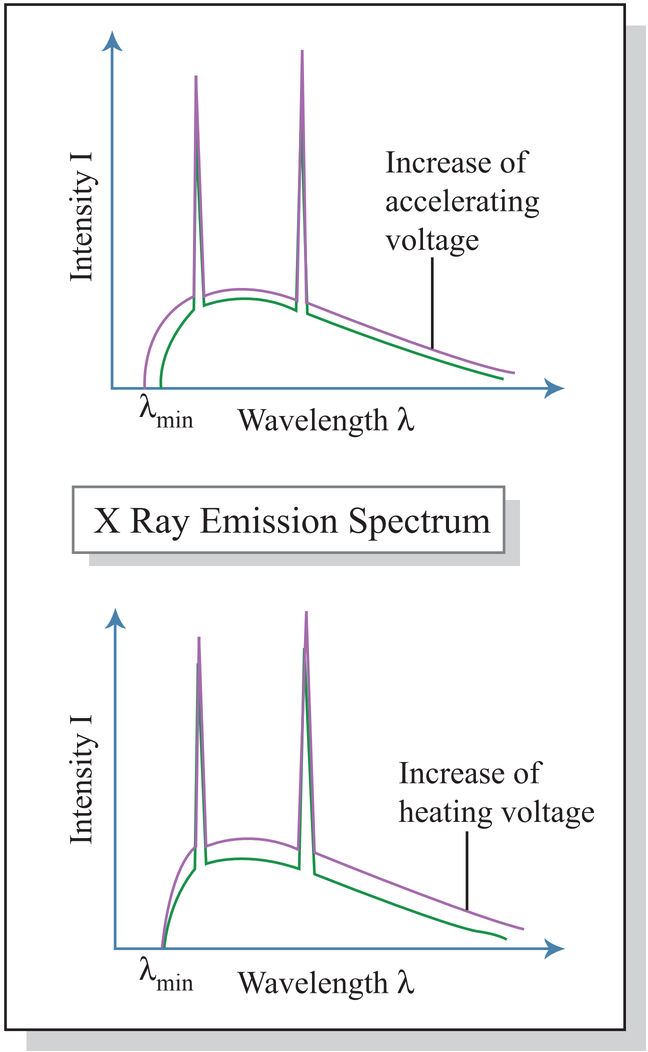


Figure by MIT OCW.

The Laue experiment

X-ray photograph of zinc blende from the Laue experiment removed for copyright reasons.
See http://capsicum.me.utexas.edu/ChE386K/html/laue_experiment.htm.

How does a crystal diffract ?

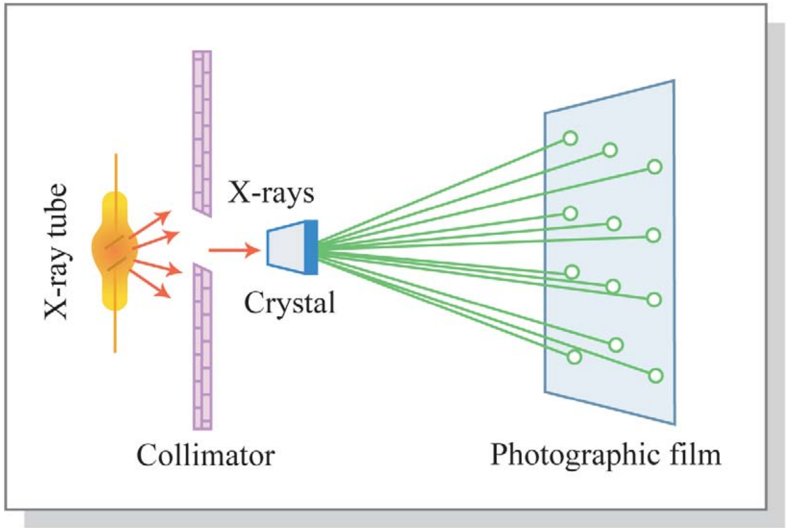
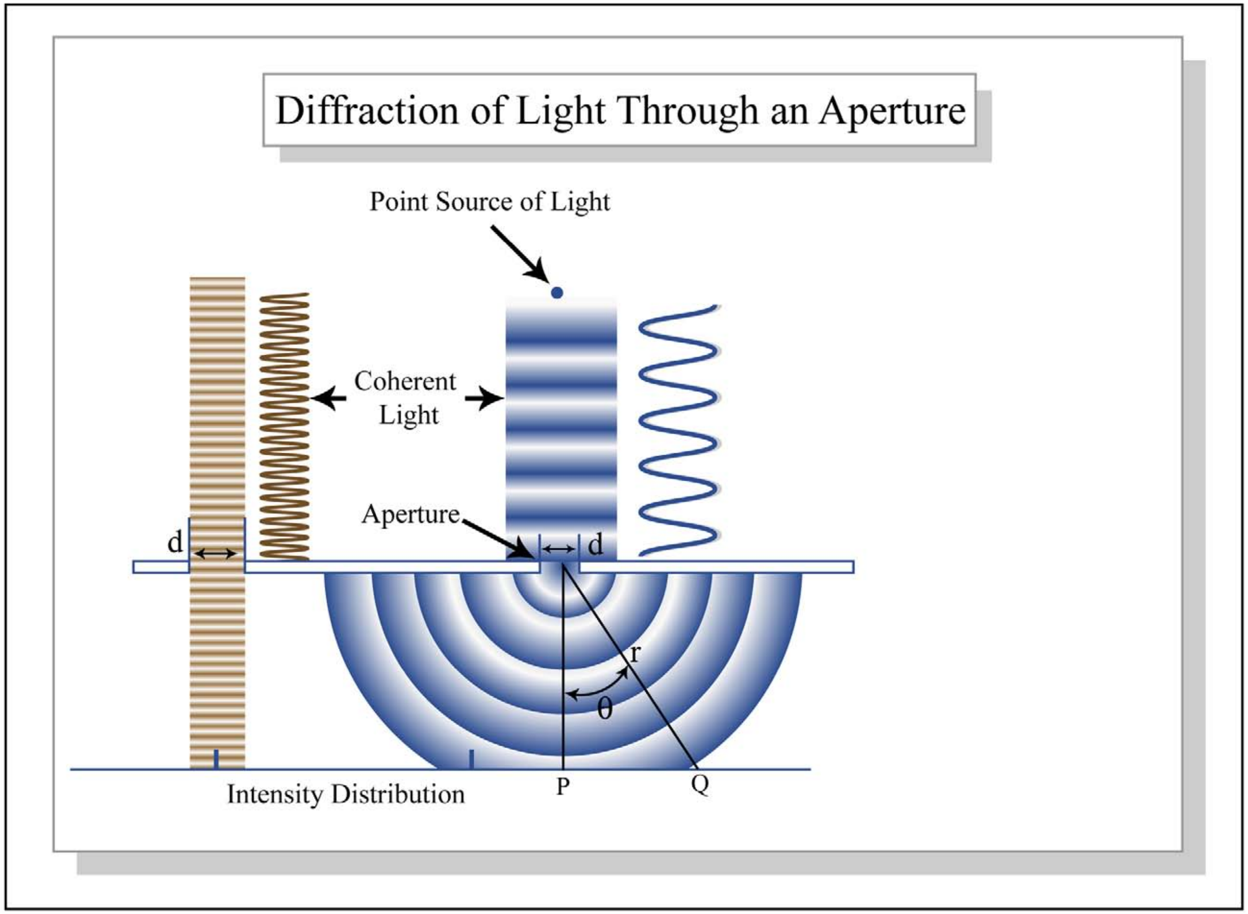


Figure by MIT OCW.

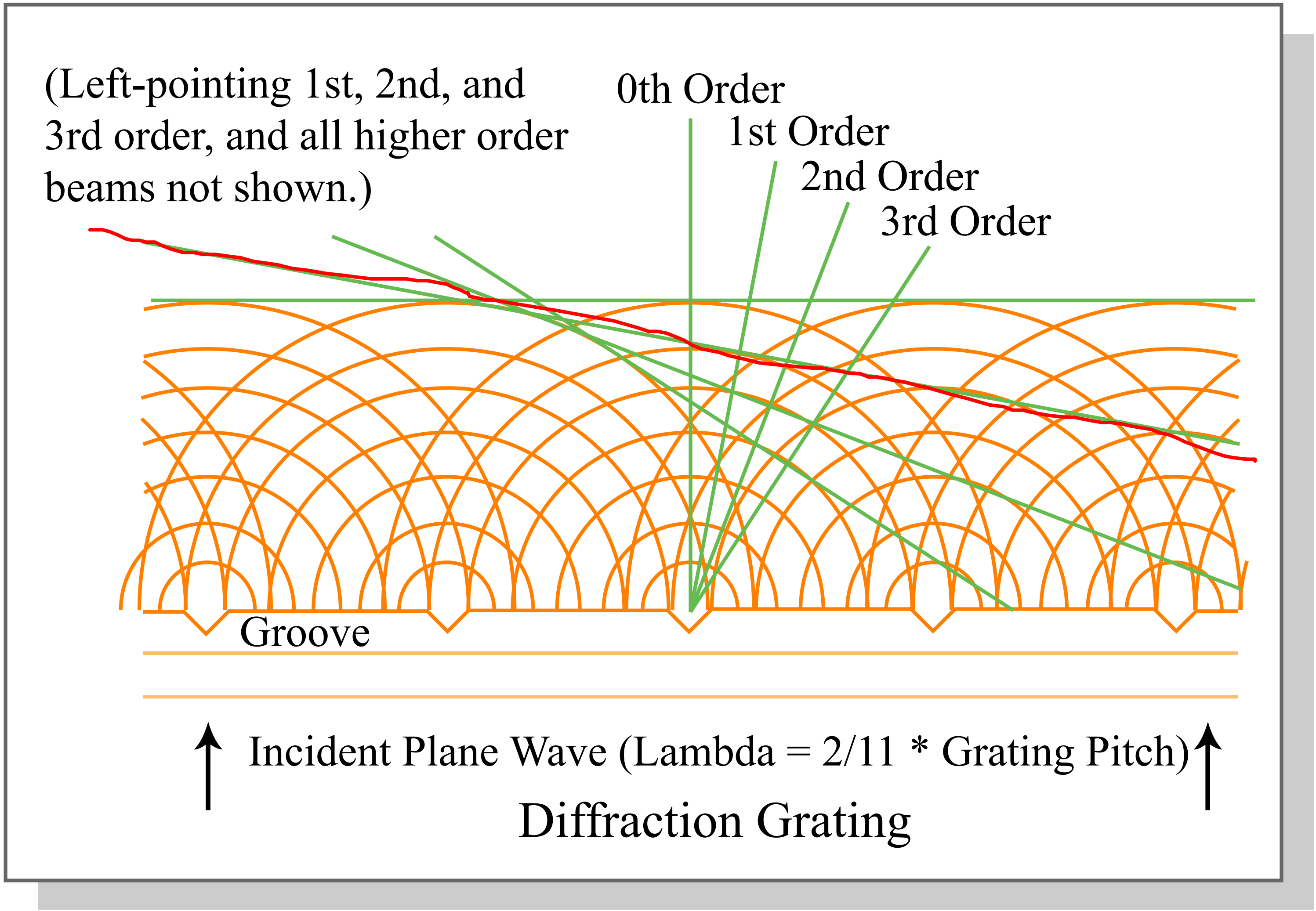
Diffraction
(wave-like instead of particle-like)



Source: Wikipedia

Figure by MIT OCW.

Diffraction from a grating



(Left-pointing 1st, 2nd, and 3rd order, and all higher order beams not shown.)

Incident Plane Wave (Lambda = 2/11 * Grating Pitch)

Diffraction Grating

Figure by MIT OCW.

Reciprocal lattice (I)

- Let's start with a Bravais lattice, defined in terms of its primitive lattice vectors…

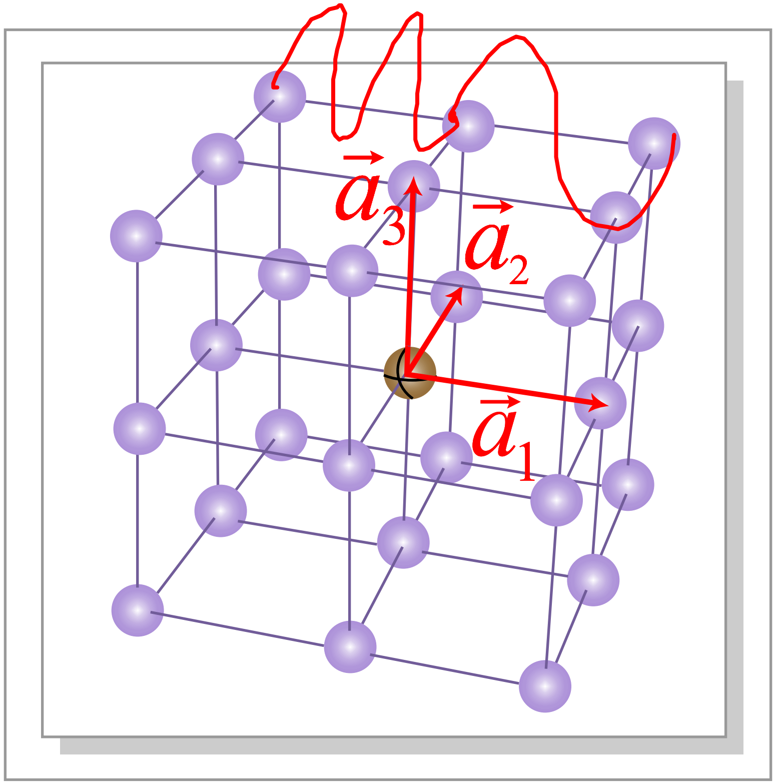


Figure by MIT OCW.

$\vec{a}_1 = (a,0,0)$ $\vec{a}_2 = (0,a,0)$ $\vec{a}_3 = (0,0,a)$

$$\vec{R} = l\vec{a}_1 + m\vec{a}_2 + n\vec{a}_3$$

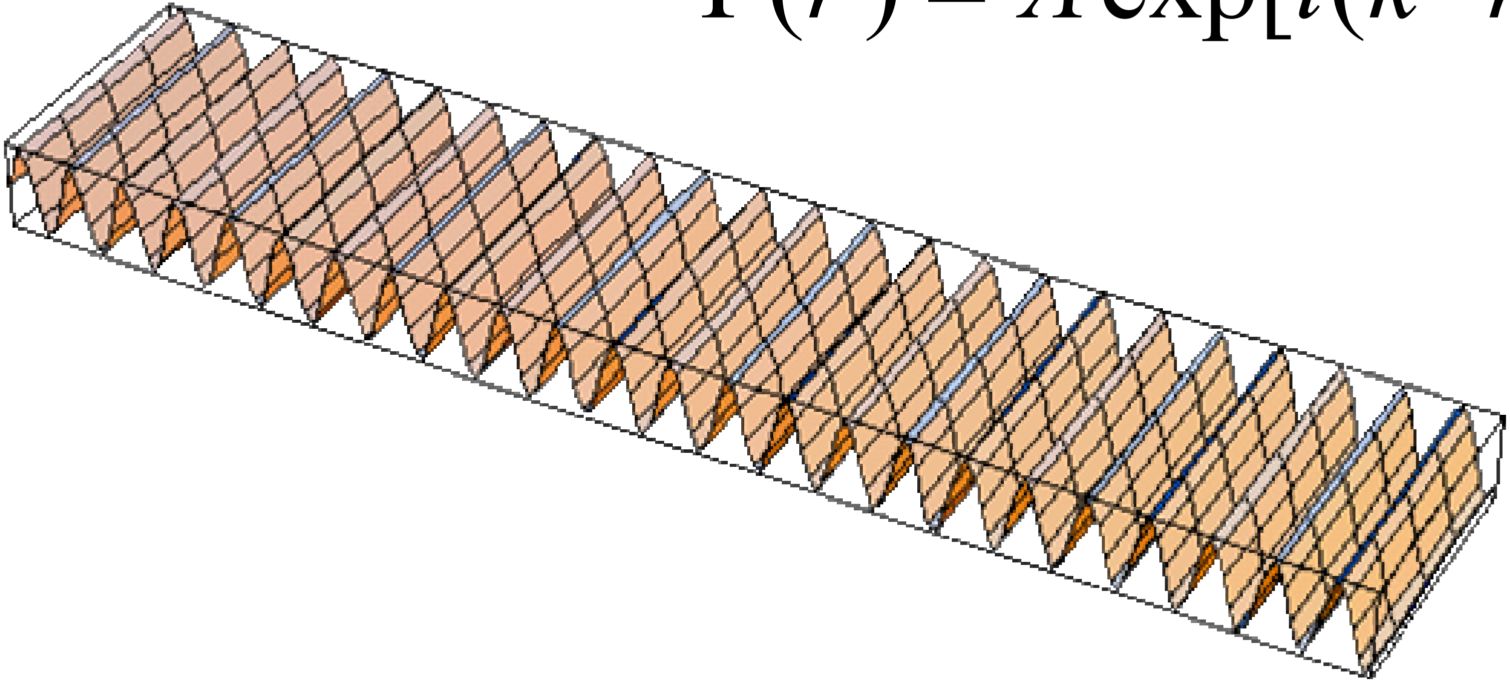
l, m, n integer numbers

$$\vec{R} = (l, m, n)$$

Reciprocal lattice (II)

- …and then let's take a plane wave

$$\Psi(\vec{r}) = A\exp[i(\vec{k}\cdot\vec{r})]$$



Reciprocal lattice (III)

- What are the wavevectors for which our plane wave has the same amplitude at all lattice points ?

$$\underbrace{A e^{i(\vec{k}\cdot\vec{r})}}_{\text{AMPLITUDE IN } \vec{r}} = \underbrace{A e^{i(\vec{k}\cdot(\vec{r}+\vec{R}))}}_{\text{AMPLITUDE IN } \vec{r}+\vec{R}}$$

SATISFIED IF $\underbrace{e^{i\vec{k}\cdot\vec{R}} = 1}$

$$\boxed{\vec{k}\cdot\vec{R} = 2\pi n}$$

Reciprocal lattice (IV)

$\vec{k}\cdot\vec{R} = 2n\pi$ n integer is satisfied by

$\vec{G} = h\vec{b}_1 + i\vec{b}_2 + j\vec{b}_3$ with h,i,j integers,

provided $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot\left(\vec{a}_2\times\vec{a}_3\right)}$ $\vec{b}_2 = 2\pi \dfrac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot\left(\vec{a}_2\times\vec{a}_3\right)}$ $\vec{b}_3 = 2\pi \dfrac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot\left(\vec{a}_2\times\vec{a}_3\right)}$

PRIMITIVE LATTICE VECTORS

$\vec{G} = \left(h,i,j\right)$ are the reciprocal-lattice vectors

Examples of reciprocal lattices

Direct lattice	Reciprocal lattice
Simple cubic	Simple cubic
FCC	BCC
BCC	FCC
Orthorhombic	Orthorhombic

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{a}_1 = (a, 0, 0)$$

$$\vec{a}_2 = (0, b, 0)$$

$$\vec{a}_3 = (0, 0, c)$$

$$\vec{b}_1 = \left(\frac{2\pi}{a}, 0, 0\right) \quad \vec{b}_2 = \left(0, \frac{2\pi}{b}, 0\right) \quad \vec{b}_3 = \left(0, 0, \frac{2\pi}{c}\right)$$

First Laue condition

$$(AB - CD) = a(\cos\alpha_n - \cos\alpha_0) = n_x\lambda$$

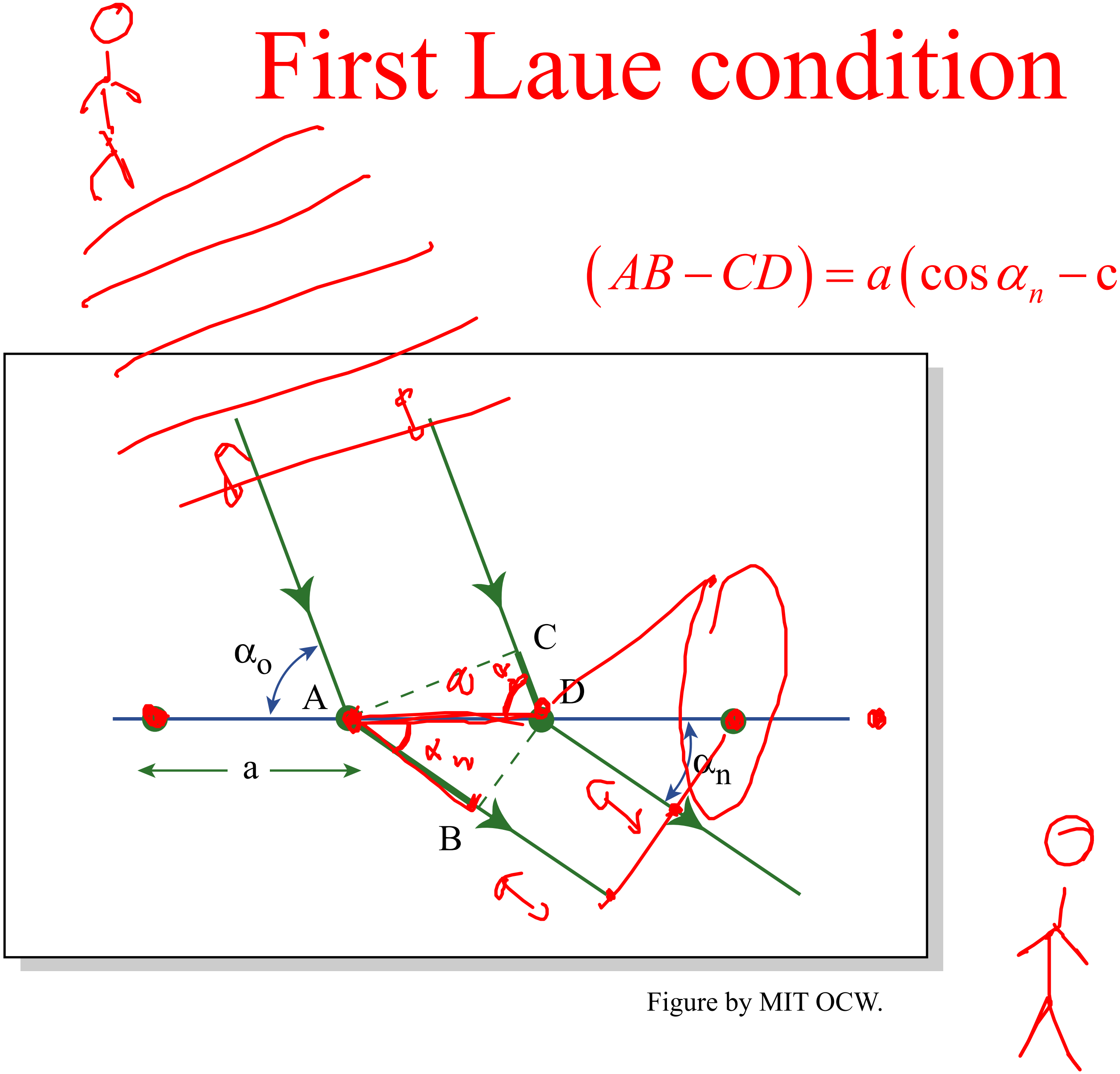
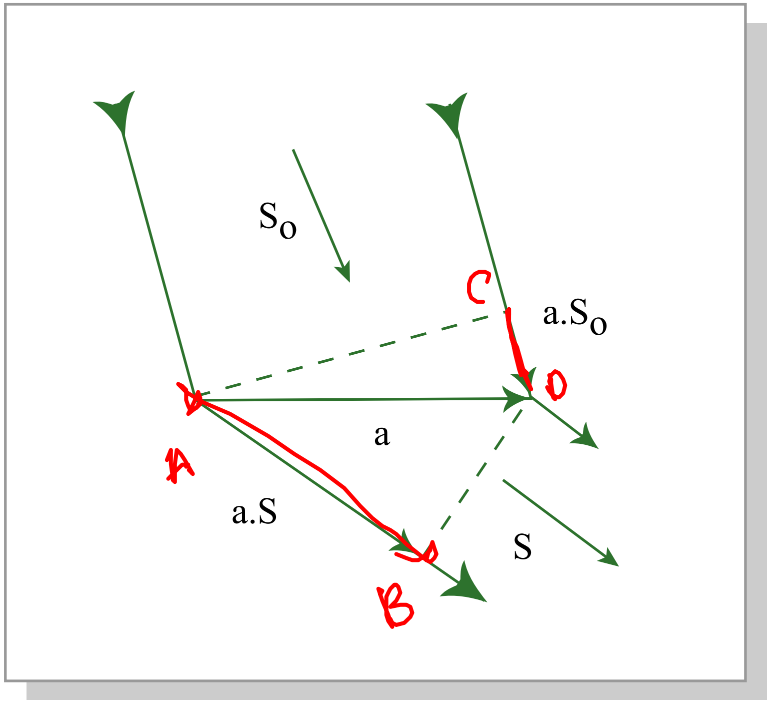


Figure by MIT OCW.

First Laue condition (vector form)



$$\vec{a}\cdot\vec{S} = a\cos\alpha_n$$

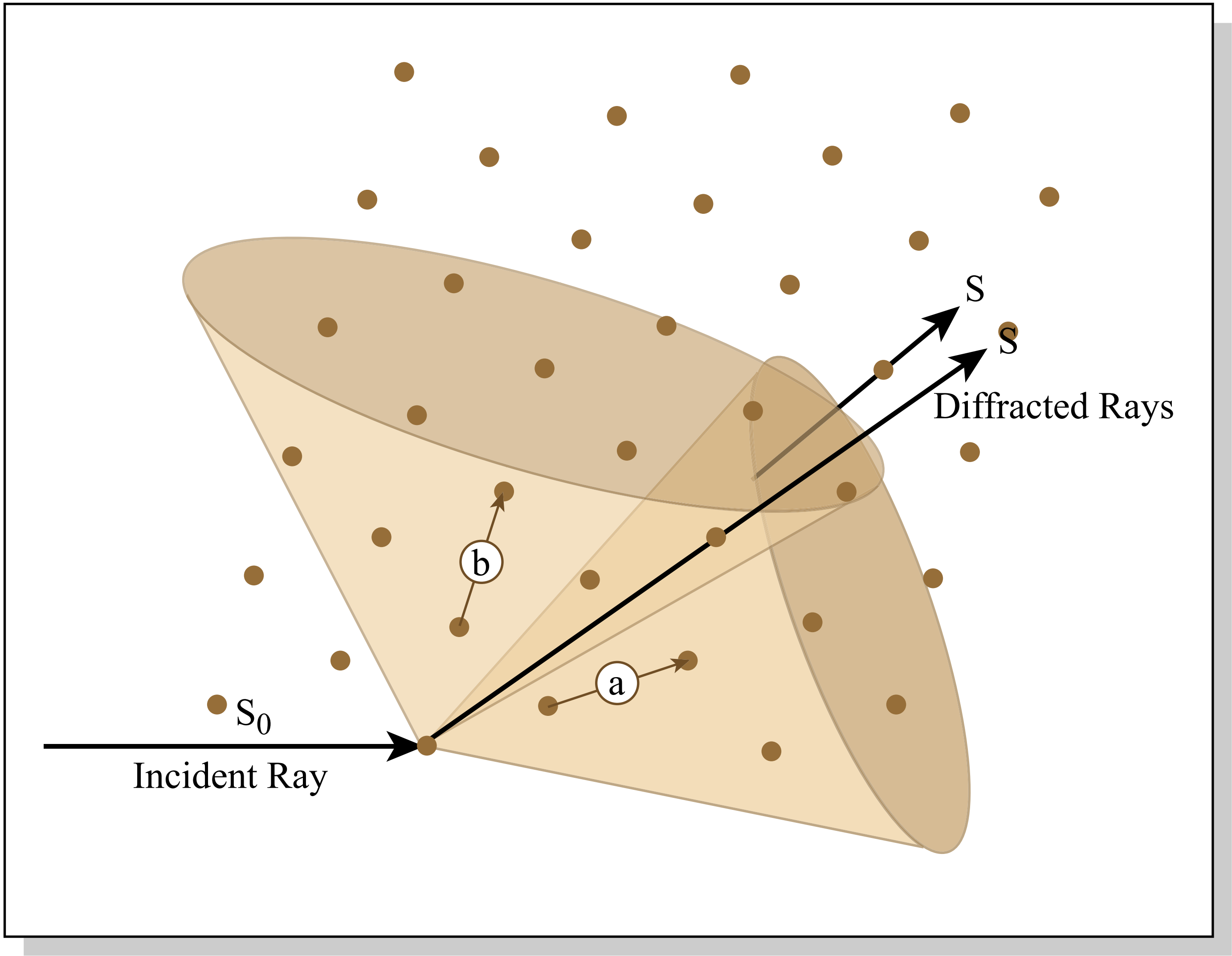
$$\vec{a}\cdot\vec{S}_0 = a\cos\alpha_0$$

$$a\left(\cos\alpha_n - \cos\alpha_0\right) = \vec{a}\cdot\left(\vec{S}-\vec{S}_0\right) = n_x\lambda$$

Figure by MIT OCW.

Second Laue condition

$$b(\cos\beta_n - \cos\beta_0) = \mathbf{b}\cdot(\mathbf{S}-\mathbf{S}_0) = n_y\lambda$$



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Third Laue condition

$$a\left(\cos\alpha_n - \cos\alpha_0\right) = \mathbf{a}\cdot\left(\mathbf{S}-\mathbf{S}_0\right) = n_x\lambda$$

$$b\left(\cos\beta_n - \cos\beta_0\right) = \mathbf{b}\cdot\left(\mathbf{S}-\mathbf{S}_0\right) = n_y\lambda$$

$$c\left(\cos\gamma_n - \cos\gamma_0\right) = \mathbf{c}\cdot\left(\mathbf{S}-\mathbf{S}_0\right) = n_z\lambda$$

PRIMITIVE
LATTICE VECTORS

Back-reflection and transmission Laue

Diagrams of the Laue Method removed for copyright reasons.
See the images at http://www.matter.org.uk/diffraction/x-ray/laue_method.htm.