

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

Last time:

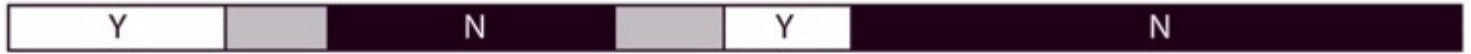
1. Glide planes, screw axes
2. Space groups
3. Bravais lattices: sc, bcc, fcc (also, lattice with a basis)
4. Primitive, conventional, and Wigner-Seitz cells
5. Miller indices
6. Diamond, zincblend, perovskites, rocksalt, CsCl

Probing with radiation

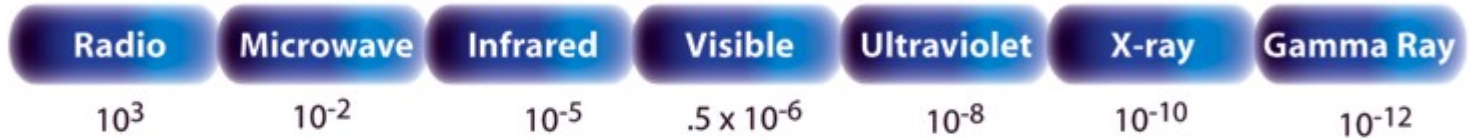
- Wavelength need to be smaller than typical interatomic distances
- Beams of photon (X-rays), electrons, neutrons
- We look at **coherent** (all same atoms behave in the same way), **elastic** (no energy is lost) **scattering**
- Elastic: diffraction. Inelastic: spectroscopies
- We “interrogate” long-range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

THE ELECTROMAGNETIC SPECTRUM

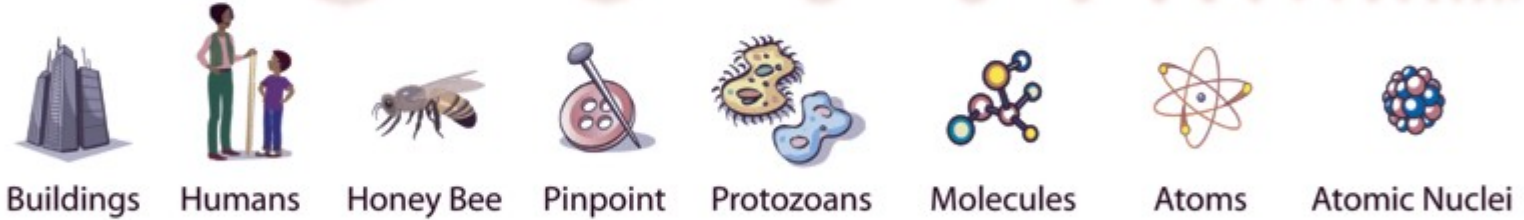
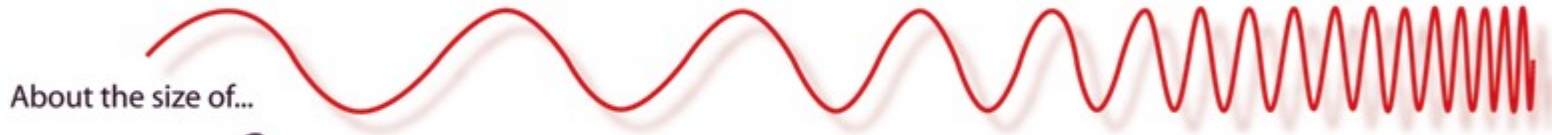
Penetrates Earth Atmosphere?



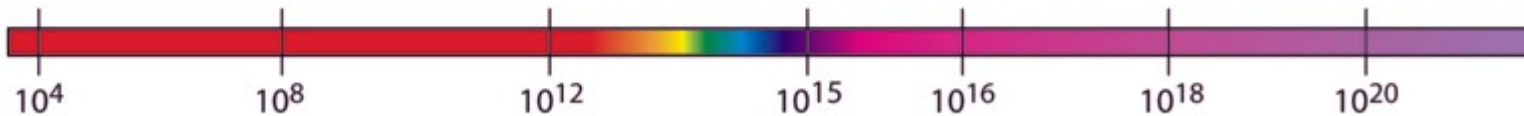
Wavelength (meters)



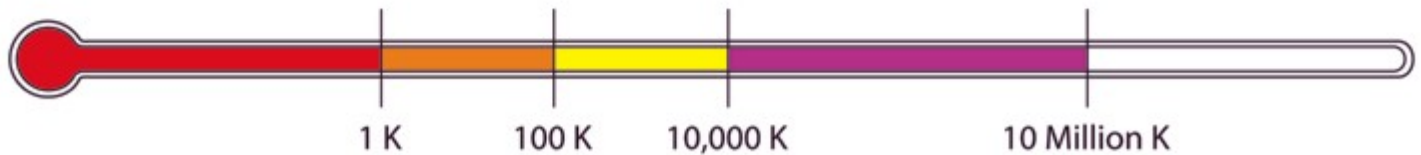
About the size of...



Frequency (Hz)



Temperature of bodies emitting the wavelength (K)



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

Energy of an accelerated electron

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

$$V = \frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{sec})(2.998 \times 10^{10} \text{ cm/sec})}{(10^{-8} \text{ cm/\AA})(1.602 \times 10^{-19} \text{ J/V})}$$
$$= 12.4 \times 10^3 \text{ V/\AA}$$

$$kV = \frac{12.4}{\lambda} \quad \lambda [=] \text{\AA}$$

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

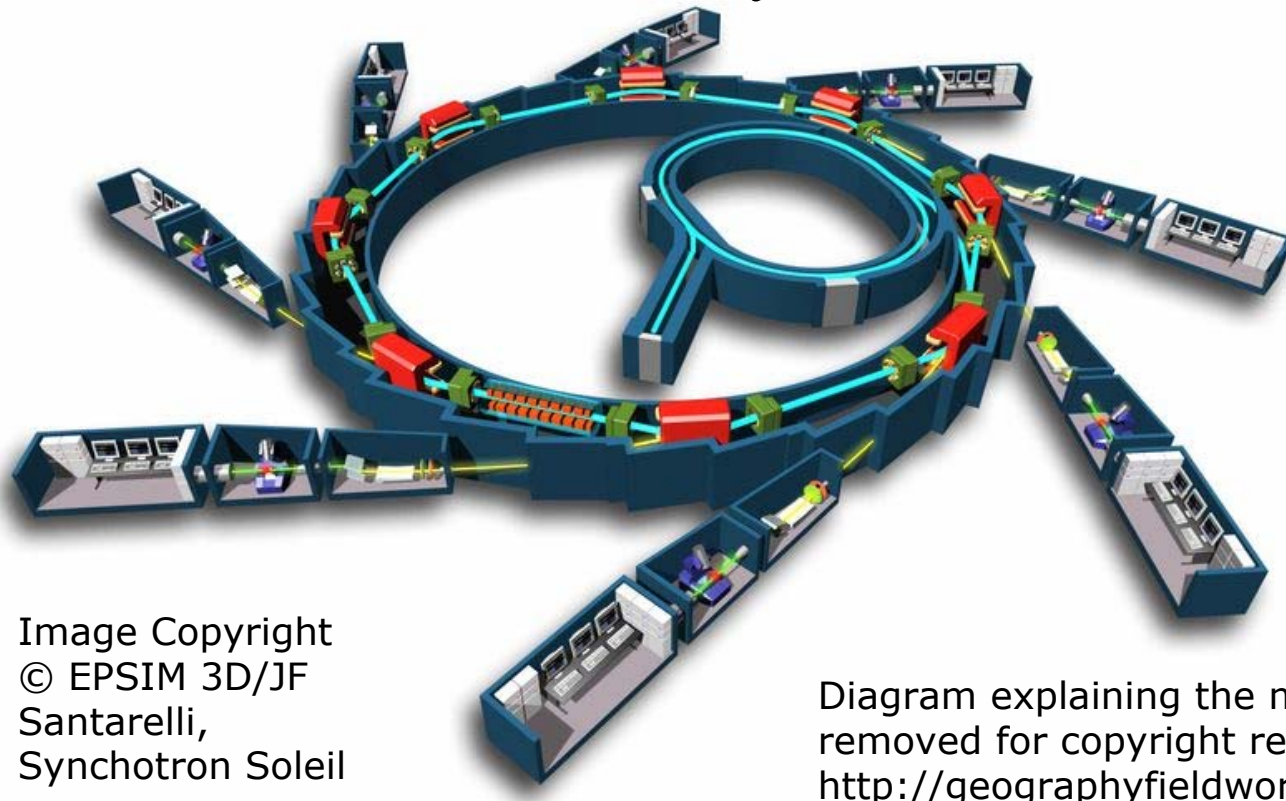


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© EPSIM 3D/JF
Santarelli,
Synchrotron Soleil

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 *Bremsstrahlung*
 - In addition, we excite core electrons, that decay back emitting radiation at K, L, M lines

Moseley law

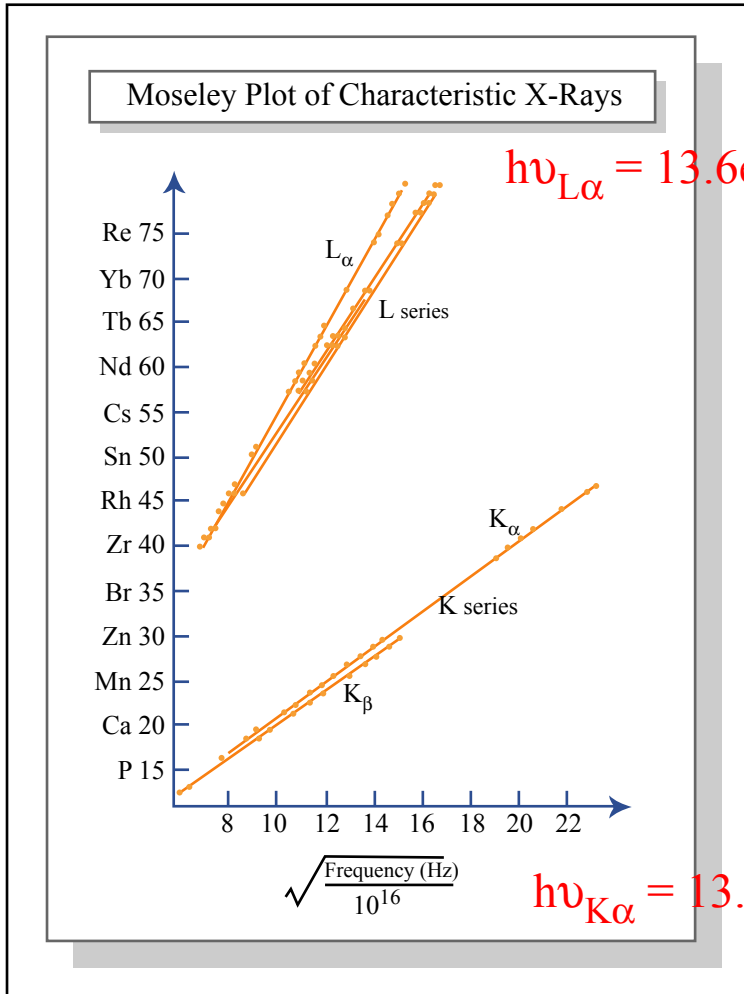


Figure by MIT OCW.

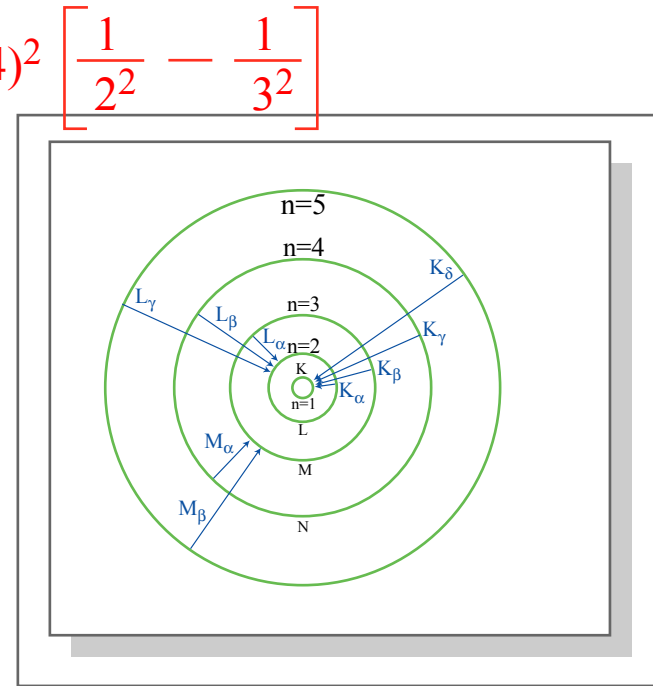


Figure by MIT OCW.

How do we generate X-rays?

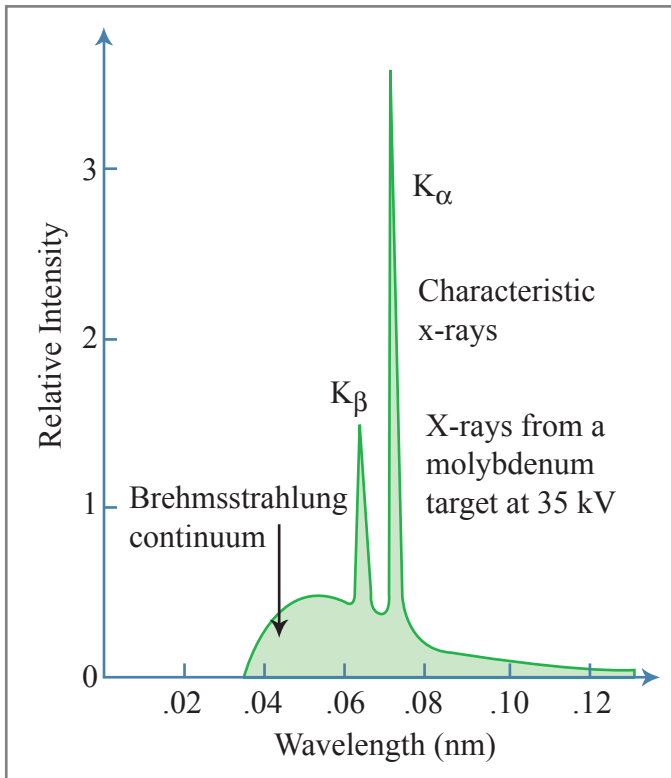


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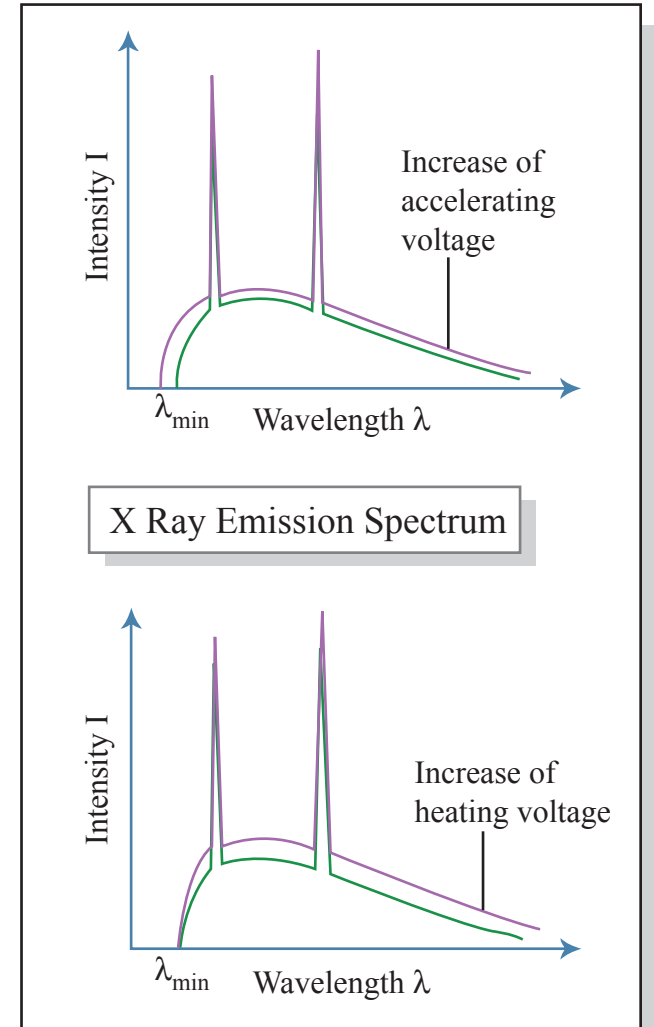


Figure by MIT OCW.

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 ?

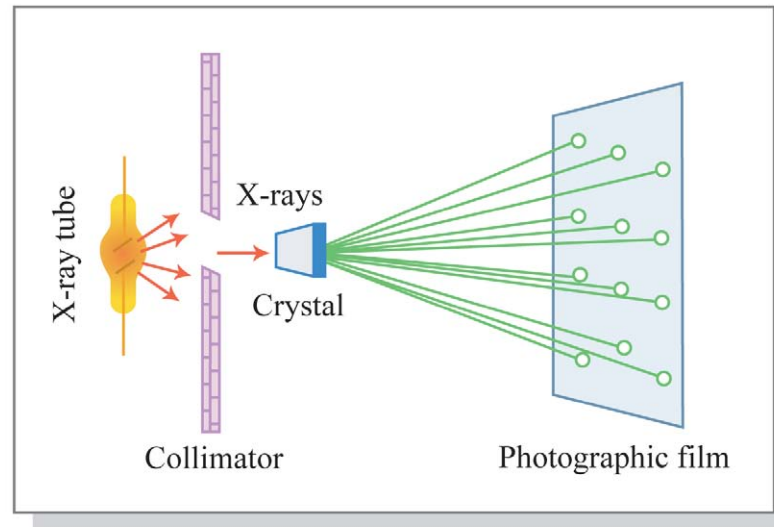


Figure by MIT OCW.

Diffraction (wave-like instead of particle-like)

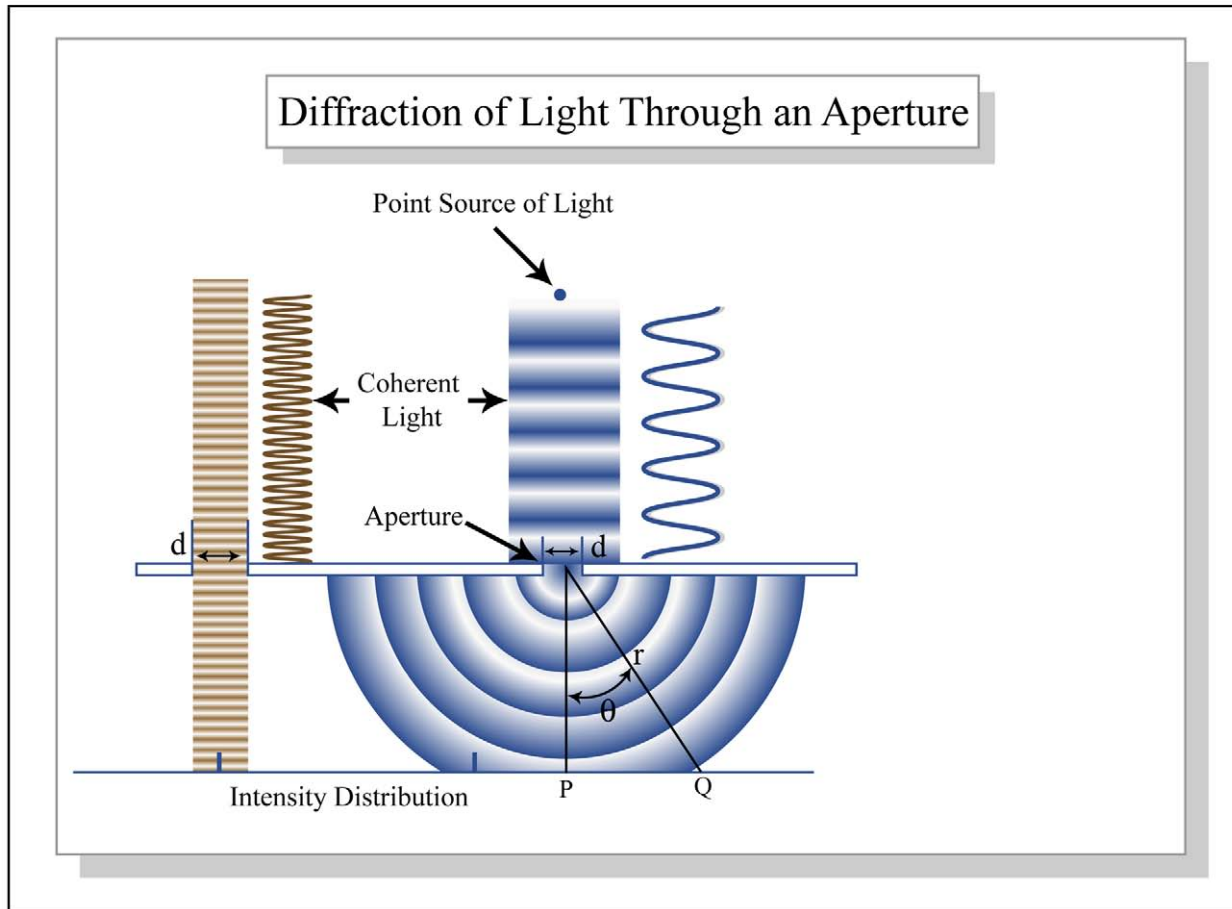


Figure by MIT OCW.



Source: Wikipedia

Figure by MIT OCW.

Diffraction from a grating

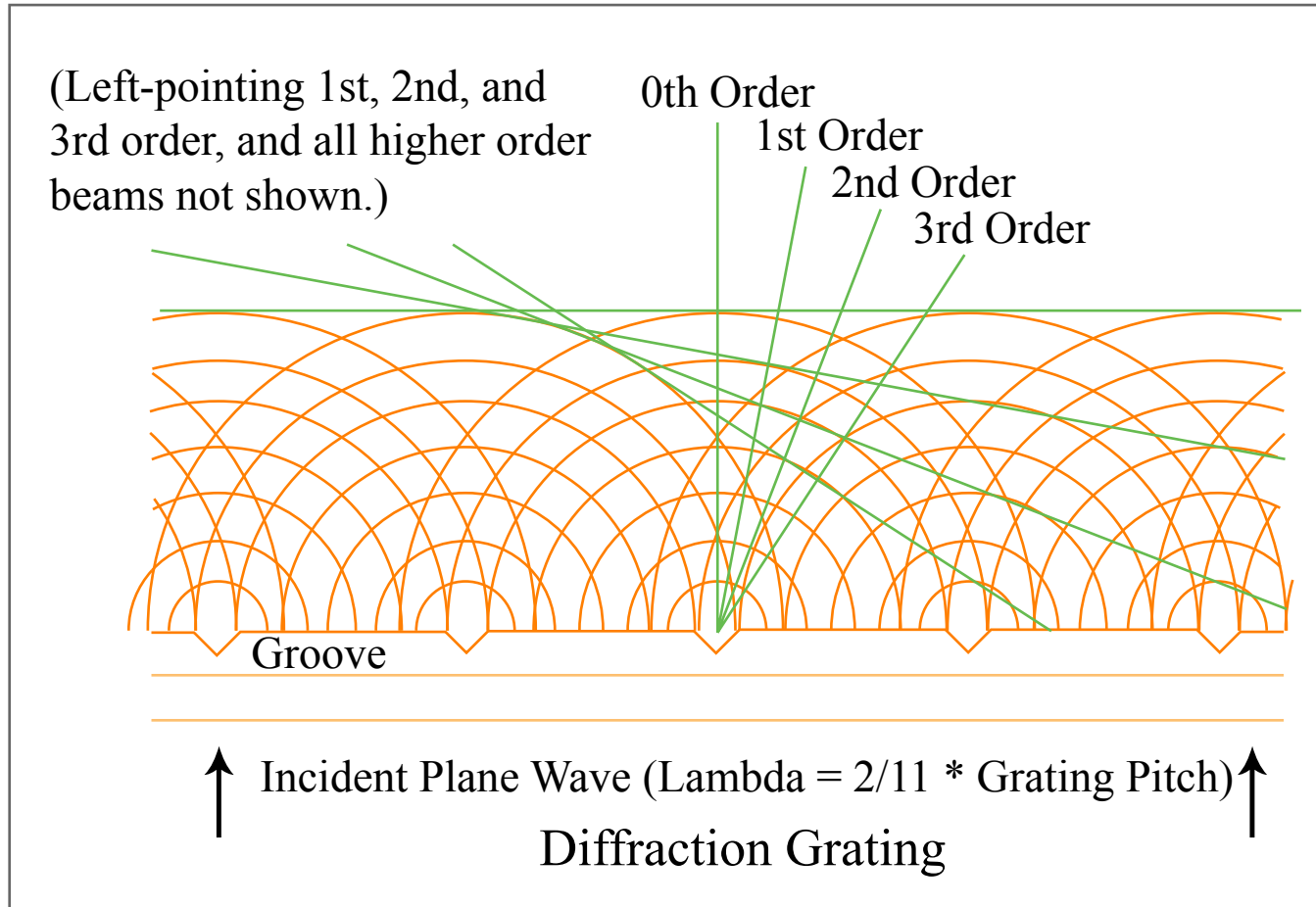
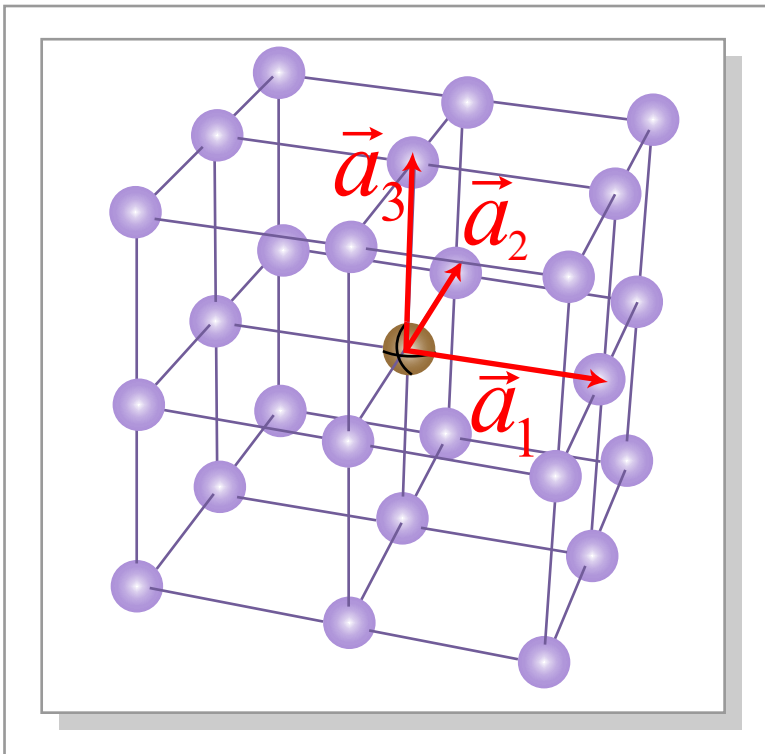


Figure by MIT OCW.

Reciprocal lattice (I)

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



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

l, m, n integer numbers

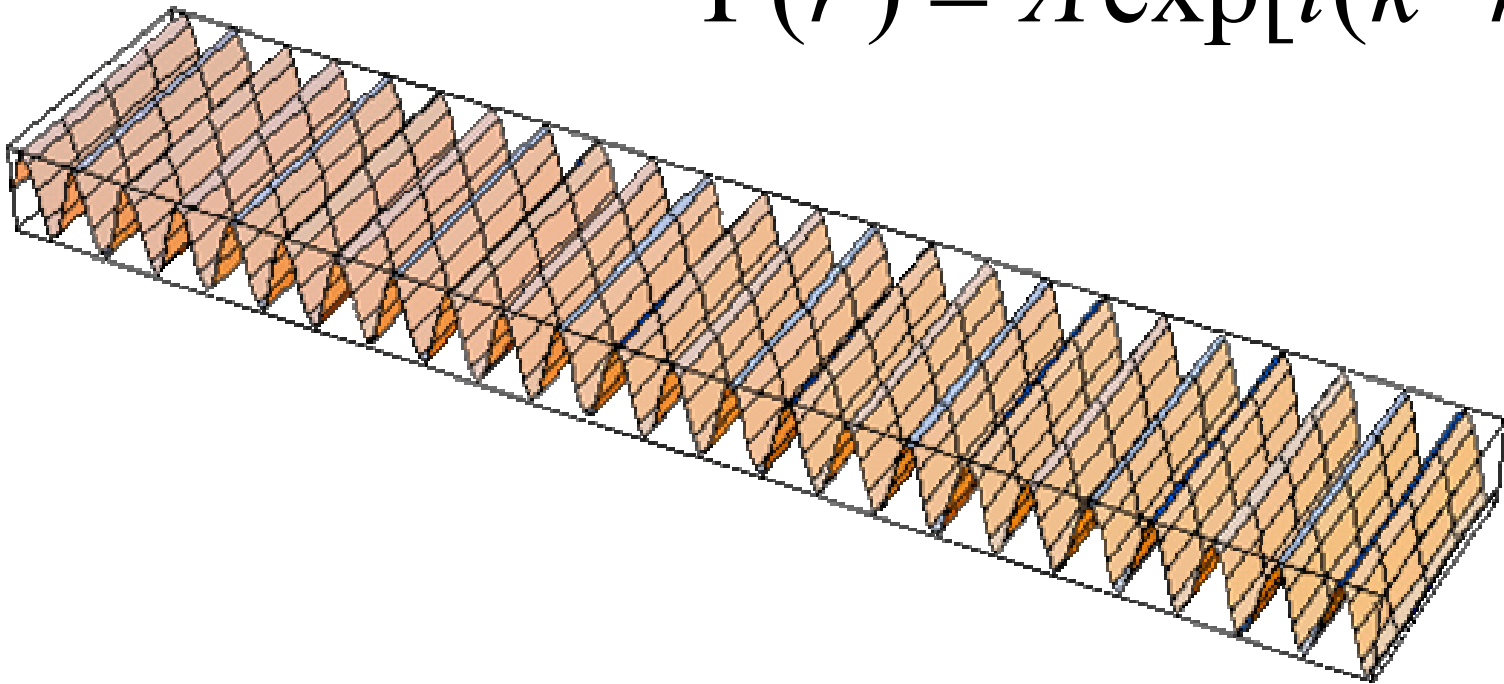
$$\vec{R} = (l, m, n)$$

Figure by MIT OCW.

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 ?

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

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

Examples of reciprocal lattices

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

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

First Laue condition

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

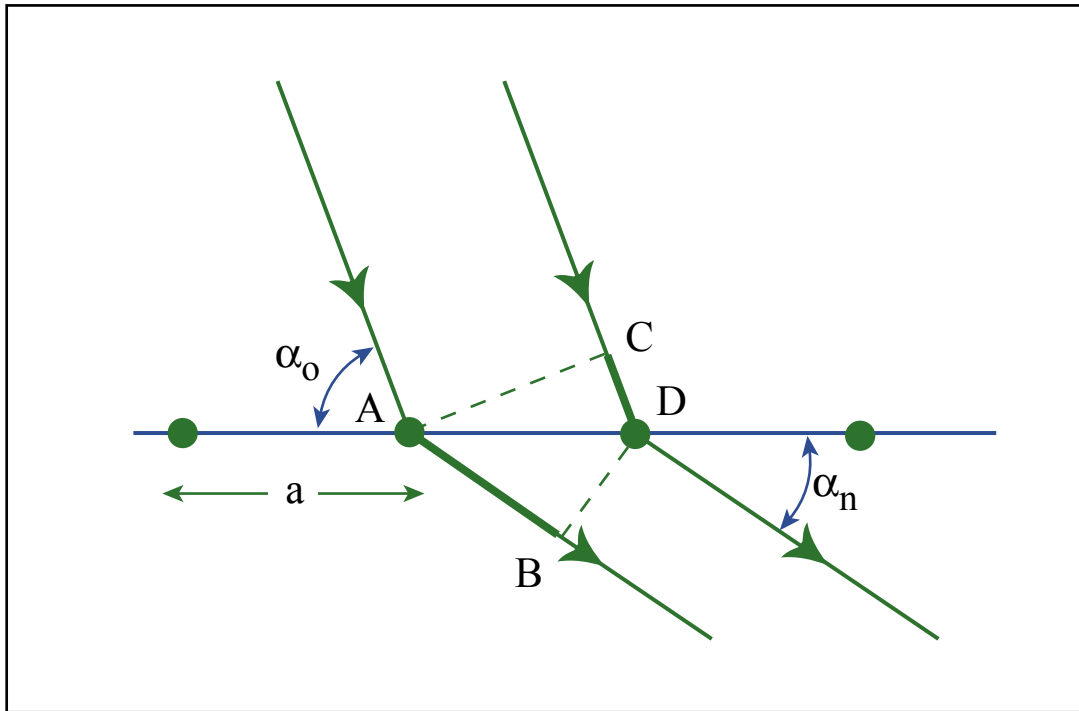


Figure by MIT OCW.

First Laue condition (vector form)

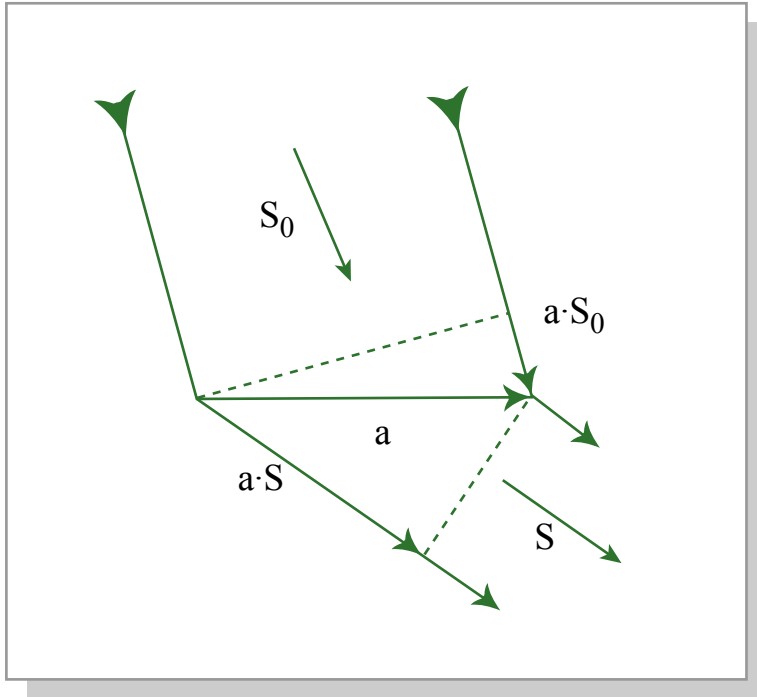


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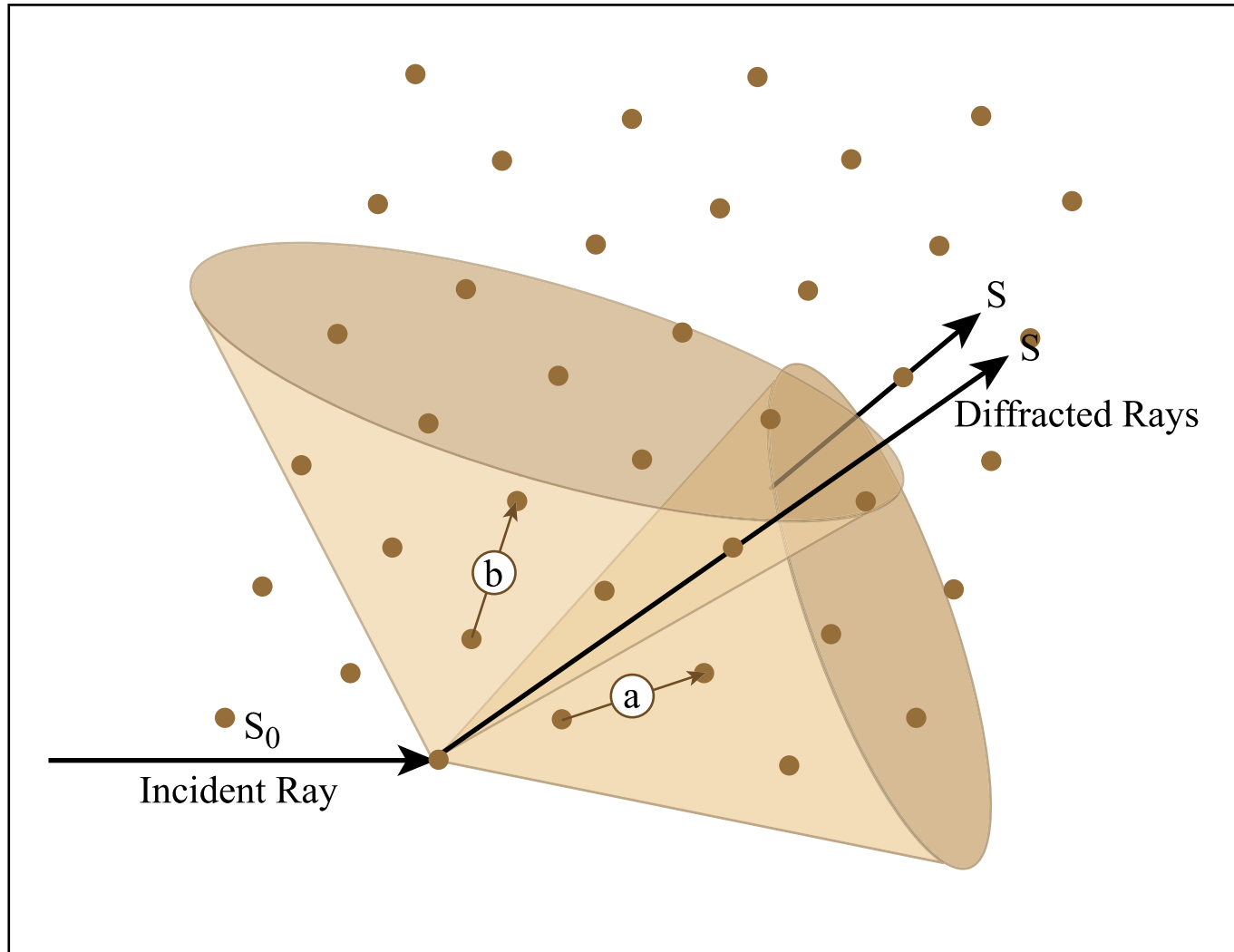
$$\vec{a} \cdot \vec{S} = a \cos \alpha_n$$

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

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

Second Laue condition

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



Third Laue condition

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

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

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

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.