CHAPTER 3
X-RAY DIFFRACTION IN CRYSTAL

I. X-Ray
II. Diffraction
III. Diffraction of Waves by Crystals
IV. X-Ray Diffraction
V. Bragg Equation
VI. X-Ray Methods
VII. Neutron & Electron Diffraction

Bertha Röntgen's Hand 8 Nov, 1895

X-RAY

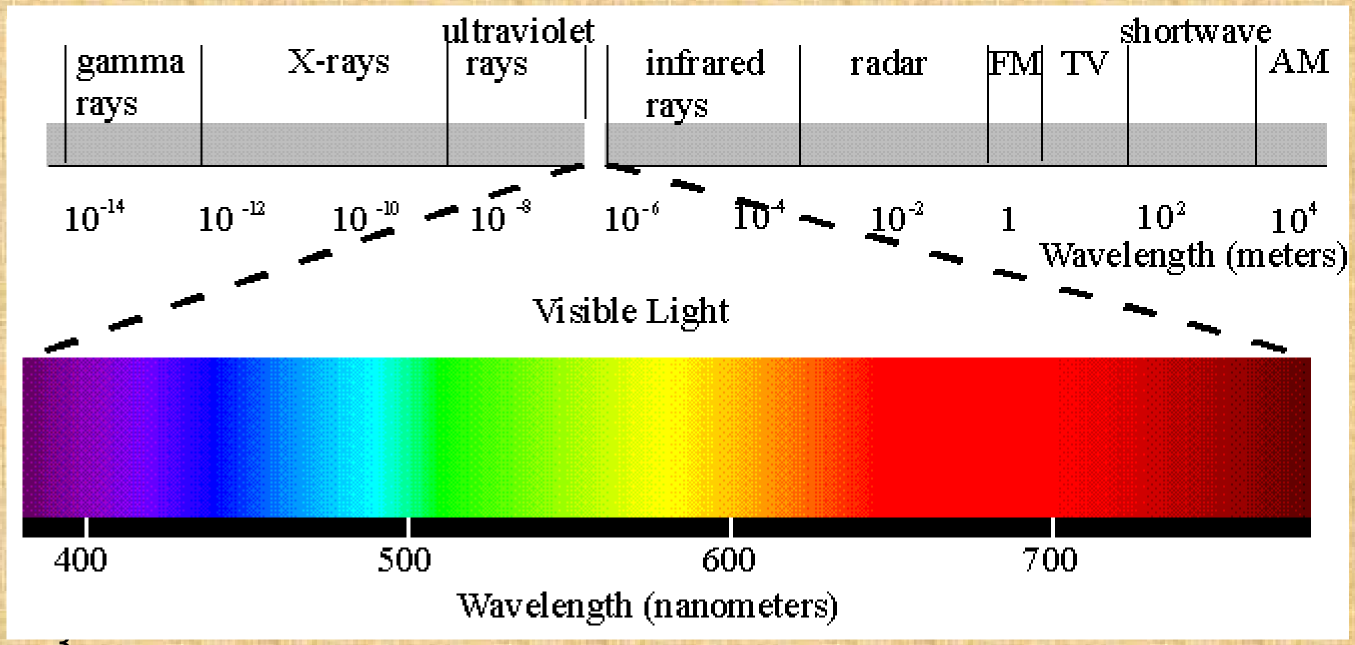
- X-rays were discovered in 1895 by the German physicist Wilhelm Conrad Röntgen and were so named because their nature was unknown at the time.

- He was awarded the Nobel prize for physics in 1901.

Wilhelm Conrad Röntgen
(1845-1923)

X-RAY PROPERTIES

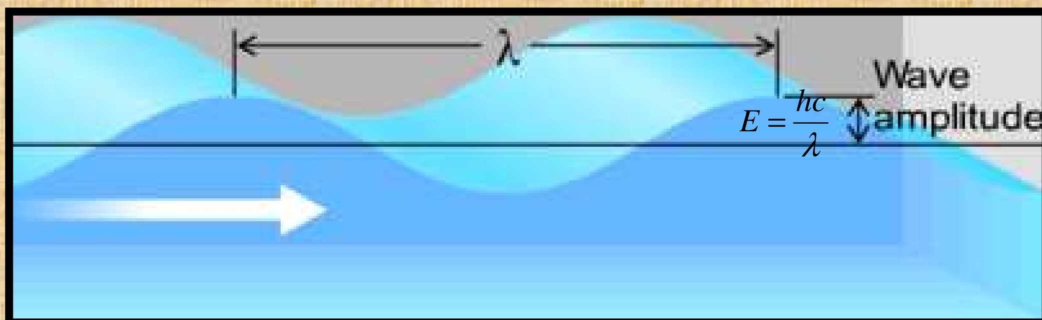
- X ray, invisible, highly penetrating electromagnetic radiation of much shorter wavelength (higher frequency) than visible light. The wavelength range for X rays is from about 10^{-8} m to about 10^{-11} m, the corresponding frequency range is from about 3×10^{16} Hz to about 3×10^{19} Hz.



X-RAY ENERGY

- Electromagnetic radiation described as having packets of energy, or photons. The energy of the photon is related to its frequency by the following formula:

$$E = h\nu$$



$$\nu = \frac{c}{\lambda}$$

$$E = \frac{hc}{\lambda}$$

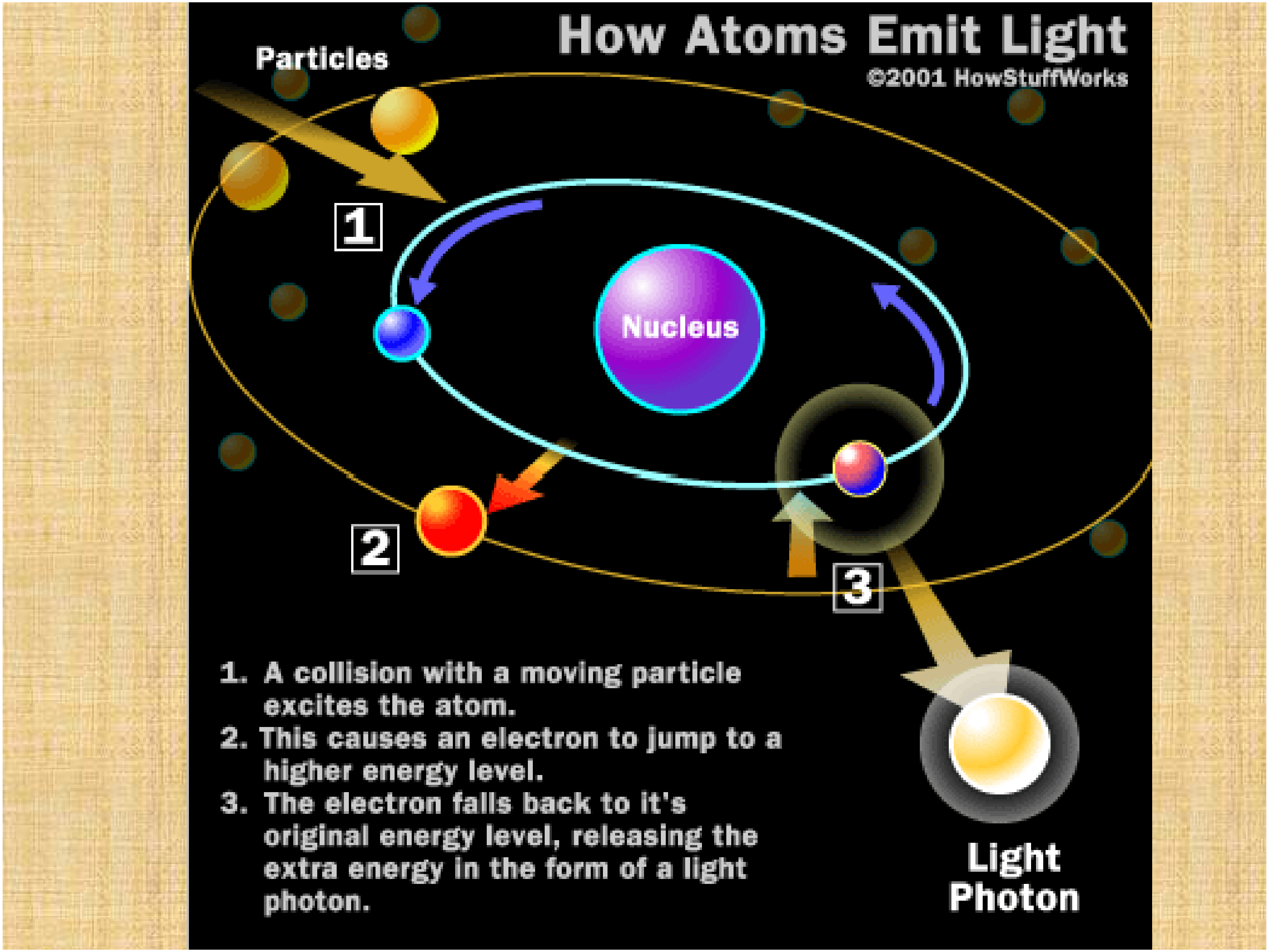
λ=Wavelength , ν = Frequency , c = Velocity of light

$$\lambda_{\text{x-ray}} \approx 10^{-10} \approx 1A^{\circ} \longrightarrow E \simeq 10^{4}\ \text{ev}$$

PRODUCTION OF X-RAYS

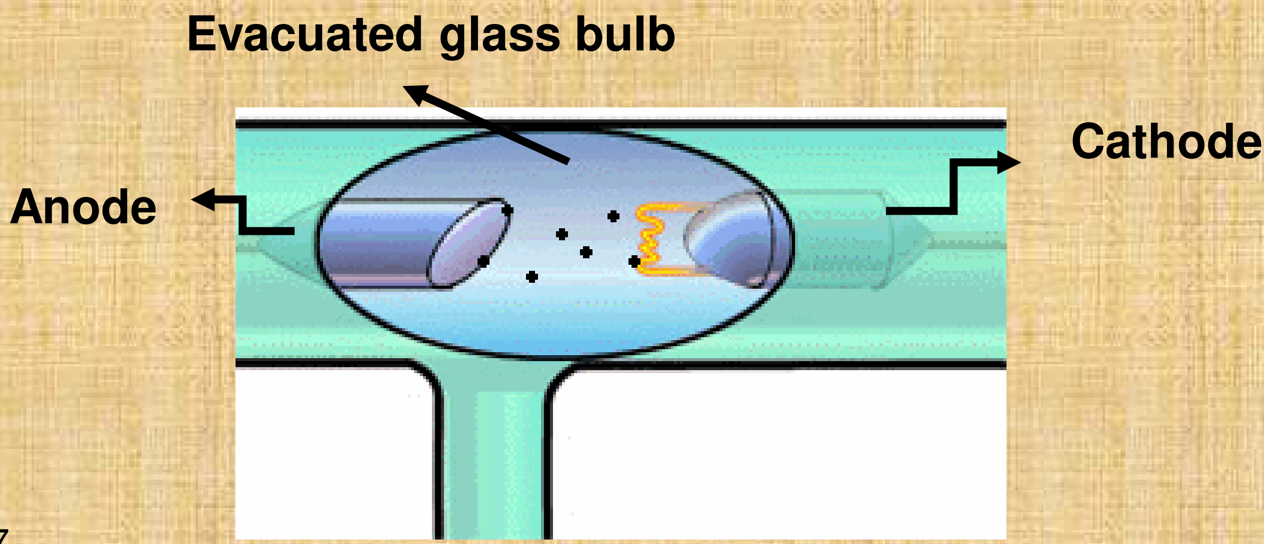
- Visible light photons and X-ray photons are both produced by the movement of **electrons** in atoms. Electrons occupy different energy levels, or orbitals, around an atom's nucleus.

- When an electron drops to a lower orbital, it needs to release some energy; it releases the extra energy in the form of a photon. The energy level of the photon depends on how far the electron dropped between orbitals.


How Atoms Emit Light
©2001 HowStuffWorks
Particles
1
Nucleus
2
3
1. A collision with a moving particle excites the atom.
2. This causes an electron to jump to a higher energy level.
3. The electron falls back to it's original energy level, releasing the extra energy in the form of a light photon.
Light Photon

X-RAY TUBE

- X rays can be produced in a highly evacuated glass bulb, called an X-ray tube, that contains essentially two electrodes—an anode made of platinum, tungsten, or another heavy metal of high melting point, and a cathode. When a high voltage is applied between the electrodes, streams of electrons (cathode rays) are accelerated from the cathode to the anode and produce X rays as they strike the anode.



Monochromatic and Broad Spectrum of X-rays

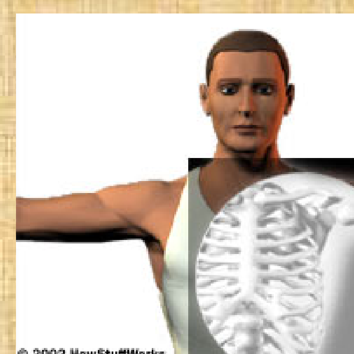
- X-rays can be created by bombarding a metal target with high energy (> 10^4) electrons.
- Some of these electrons excite electrons from core states in the metal, which then recombine, producing highly monochromatic X-rays. These are referred to as characteristic X-ray lines.
- Other electrons, which are decelerated by the periodic potential of the metal, produce a broad spectrum of X-ray frequencies.
- Depending on the diffraction experiment, either or both of these X-ray spectra can be used. 10^4

ABSORPTION OF X-RAYS

- The atoms that make up your body tissue absorb visible light photons very well. The energy level of the photon fits with various energy differences between electron positions.

...something you won't see very often (Visible Light)

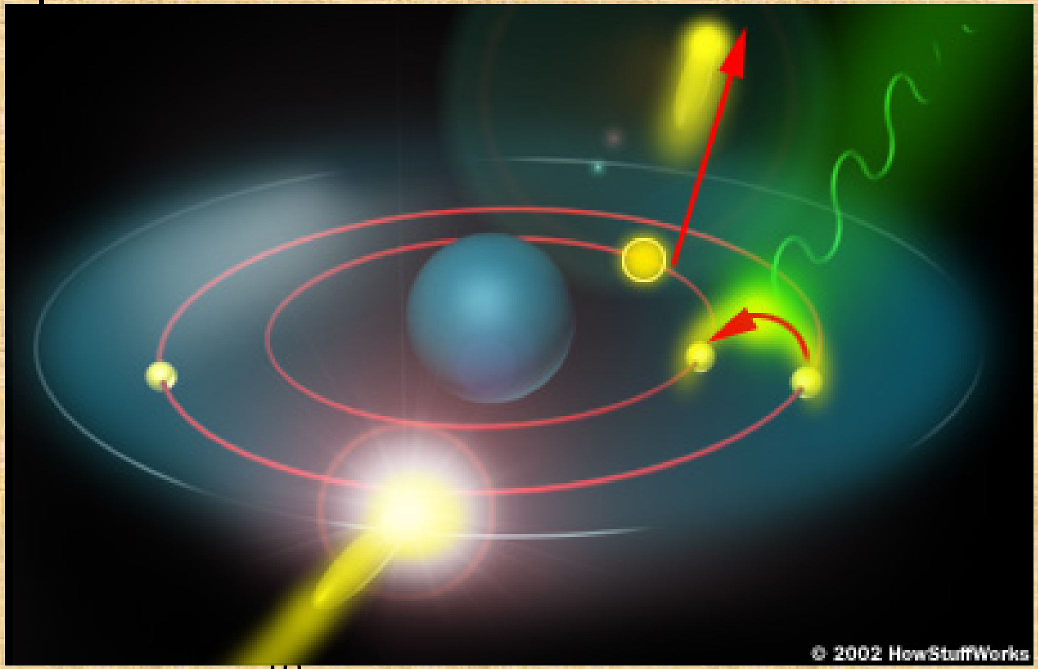
- Radio waves don't have enough energy to move electrons between orbitals in larger atoms, so they pass through most stuff. X-ray photons also pass through most things, but for the opposite reason: They have too much energy.



X-ray

Generation of X-rays (K-Shell Knockout)

An electron in a higher orbital immediately falls to the lower energy level, releasing its extra energy in the form of a photon. It's a big drop, so the photon has a high energy level; it is an X-ray photon.



The free electron collides with the tungsten atom, knocking an electron out of a lower orbital. A higher orbital electron fills the empty position, releasing its excess energy as a photon.

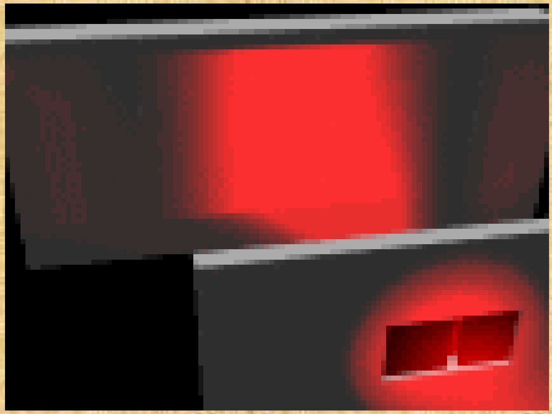
Absorption of X-rays

- A larger atom is more likely to absorb an X-ray photon in this way, because larger atoms have greater energy differences between orbitals -- the energy level more closely matches the energy of the photon. Smaller atoms, where the electron orbitals are separated by relatively low jumps in energy, are less likely to absorb X-ray photons.

- The soft tissue in your body is composed of smaller atoms, and so does not absorb X-ray photons particularly well. The calcium atoms that make up your bones are much larger, so they are better at **absorbing X-ray photons**.

DIFFRACTION

- Diffraction is a wave phenomenon in which the apparent bending and spreading of waves when they meet an obstruction.
- Diffraction occurs with electromagnetic waves, such as light and radio waves, and also in sound waves and water waves.
- The most conceptually simple example of diffraction is double-slit diffraction, that's why firstly we remember light diffraction.



Width b Variable
(500-1500 nm)

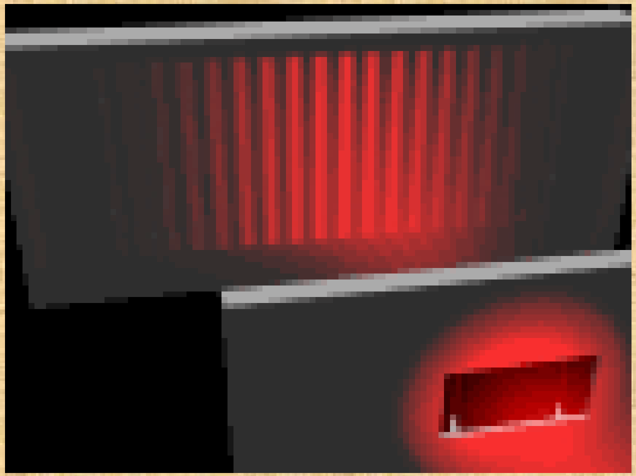
Wavelength Constant
(600 nm)

Distance d = Constant

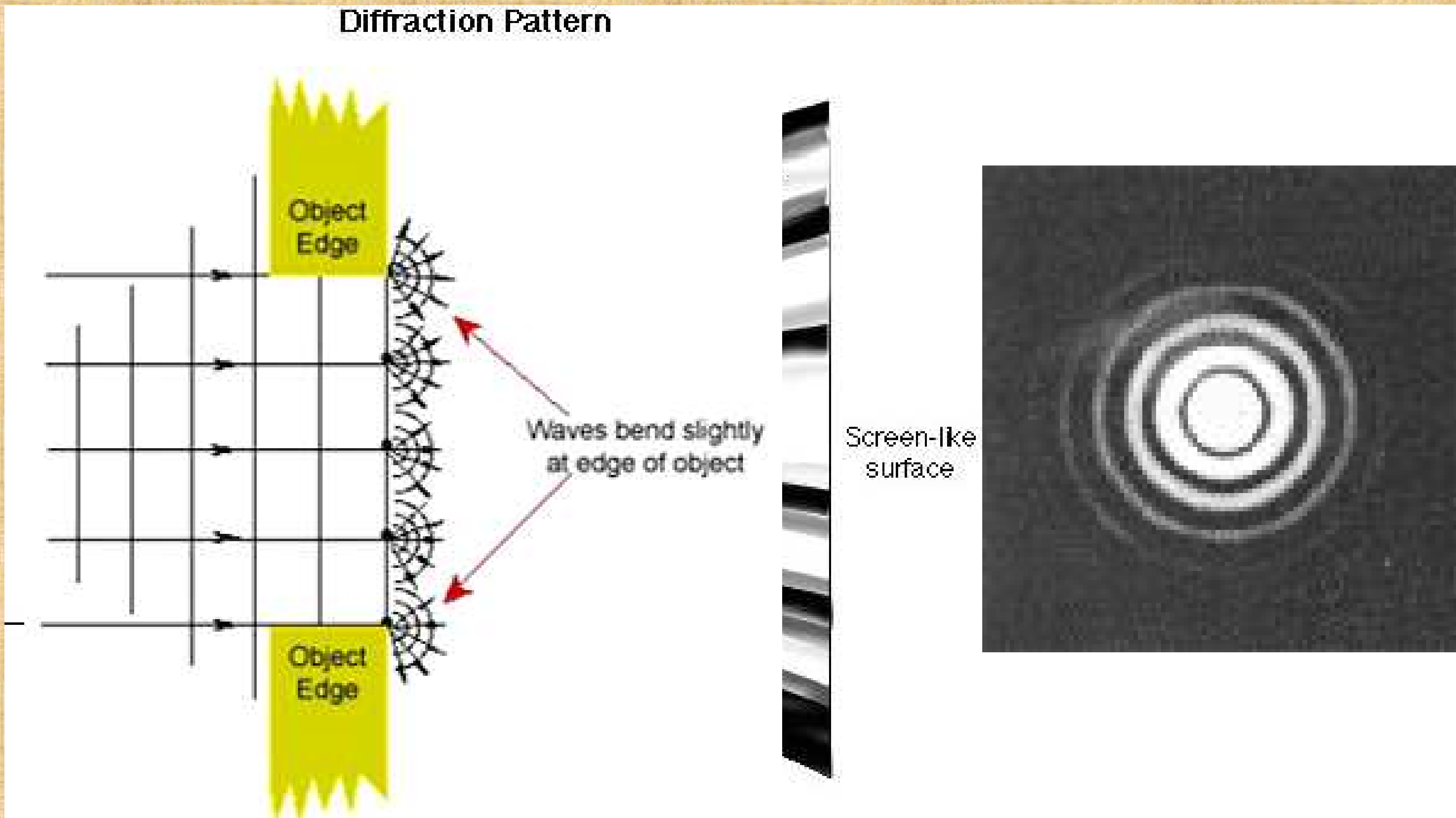
LIGHT DIFFRACTION

- Light diffraction is caused by light bending around the edge of an object. The interference pattern of bright and dark lines from the diffraction experiment can only be explained by the additive nature of waves; wave peaks can add together to make a brighter light, or a peak and a through will cancel each other out and result in darkness.

Thus Young's light interference experiment proves that light has wavelike properties.

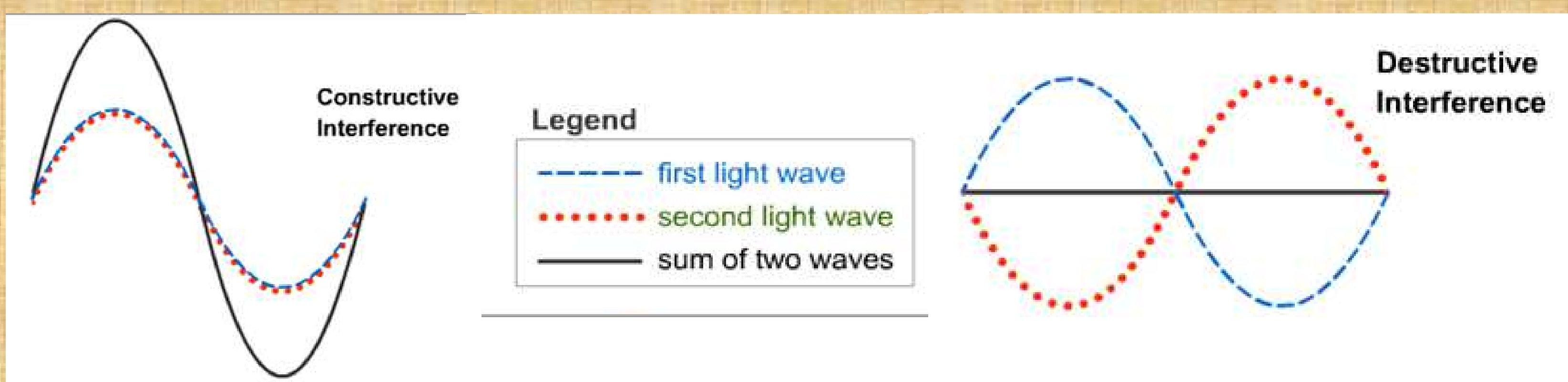


LIGHT INTERFERENCE

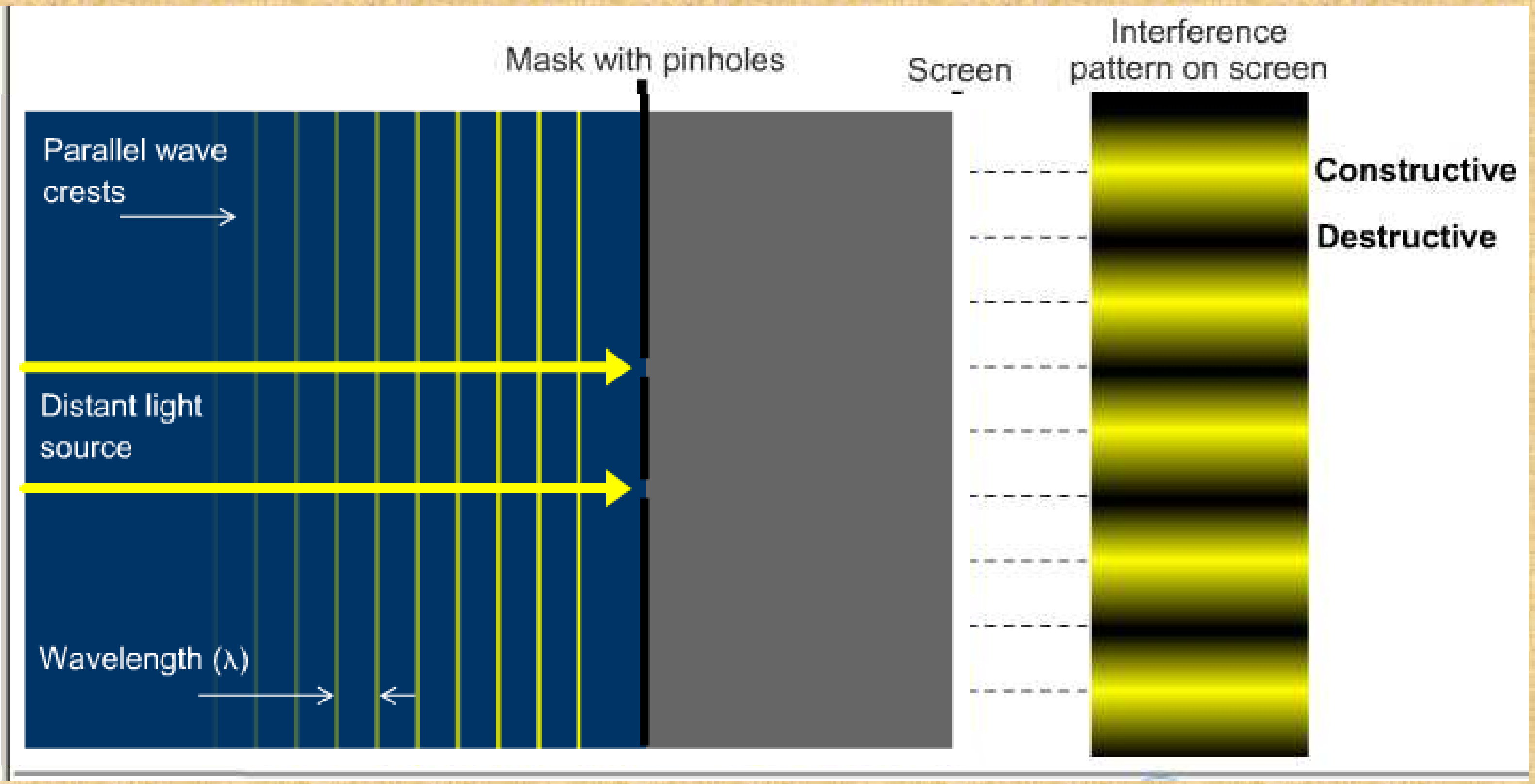


Constructive & Destructive Waves

- **Constructive interference is the result of synchronized light waves that add together to** increase **the light intensity.**
- **Destructive İnterference . results when two out-of-phase light waves cancel each other out, resulting in darkness.**



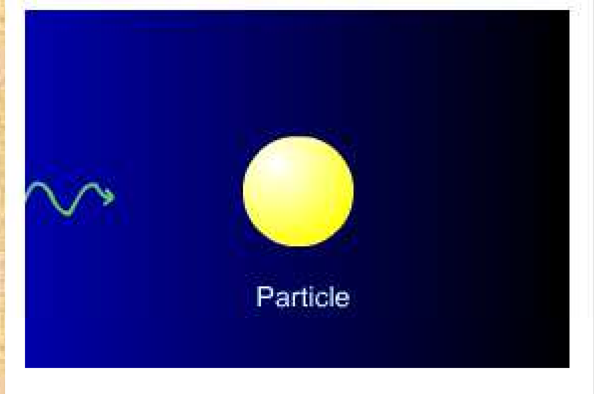
Light Interference



Diffraction from a particle and solid

Single particle

- To understand diffraction we also have to consider what happens when a wave interacts with a single particle**.** The particle scatters the incident beam uniformly in **all** directions



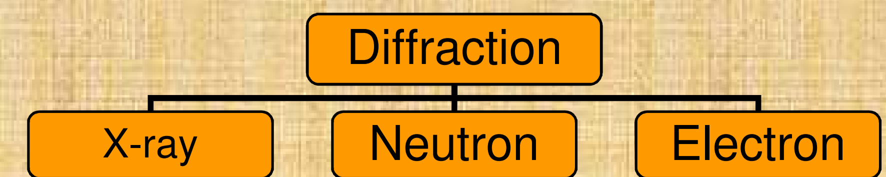
Solid material

- What happens if the beam is incident on solid material? If we consider a crystalline material, the scattered beams may add together in a few directions and reinforce each other to give **diffracted** beams

Diffraction of Waves by Crystals

A crystal is a periodic structure
(unit cells are repeated regularly)

Solid State Physics deals how the waves are propagated through such periodic structures. In this chapter we study the crystal structure through the diffraction of photons (X-ray), nuetrons and electrons.



The general princibles will be the same for each type of waves.

Diffraction of Waves by Crystals

- The diffraction depends on the crystal structure and on the wavelength.
- At optical wavelengths such as 5000 angstroms the superposition of the waves scattered elastically by the individual atoms of a crystal results in ordinary optical refraction.
- When the wavelength of the radiation is comparable with or smaller than the lattice constant, one can find diffracted beams in directions quite different from the incident radiation.

Diffraction of Waves by Crystals

- ***The structure of a crystal*** can be determined by studying the ***diffraction pattern of a*** beam of radiation incident on the crystal.

- Beam diffraction takes place ***only in certain specific directions***, much as light is diffracted by a grating.

- By measuring the ***directions of the diffraction*** and the ***corresponding intensities***, one obtains information concerning the ***crystal structure*** responsible for diffraction.