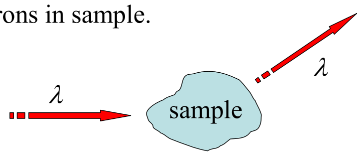
Appendix 3: X-ray diffraction (XRD)

(I) General

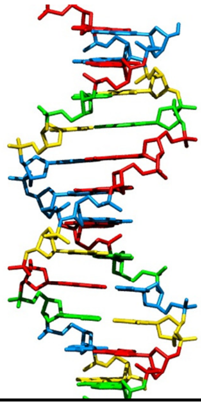
X-ray diffraction process involves only ***elastic scattering*** of x-ray photons with electrons in sample.



- It is the most important tool to characterize the crystal structure of a sample, including
  1. type of crystal structure, location of atoms in unit cell, chemical phase
  2. microstructure (single crystal/polycrystalline/amorphous, grain size,…)
  3. strain,…

- Even complicated crystal structure can be determined by x-ray diffraction.
  e.g. The double helix structure of DNA was studied in the beginning of the 1950s.

  See "The Discovery of the Molecular Structure of DNA – The Double Helix" at http://nobelprize.org/educational_games/medicine/dna_double_helix/readmore.html

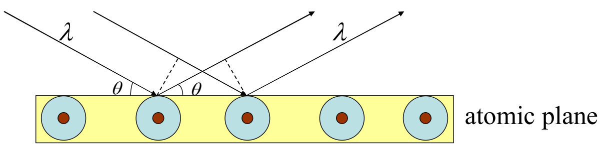


(II) Principle

(A) X-ray photon scattered by an electron (see Cullity, ch.3)
It is an elastic scattering (first studied by J.J. Thomson)
(Note: Compton scattering is inelastic.)

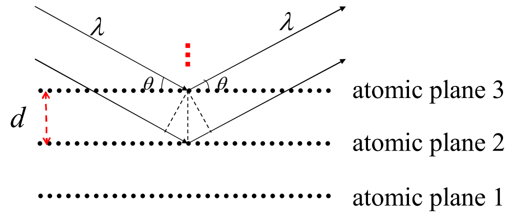
(B) X-ray photon scattered by an atom
- scattered elastically & coherently by all electrons
- not scattered by nucleus because of its heavy mass

(C) X-ray photon scattered by a plane of atoms in a lattice



Just like a mirror, incident angle = reflection angle = θ
There is no path difference in the two rays. So the two rays have the same phase. The reflection (or ***diffraction***) intensity depends on the distribution of atoms in the plane and the electron clouds of the atom(s) and the angle θ.

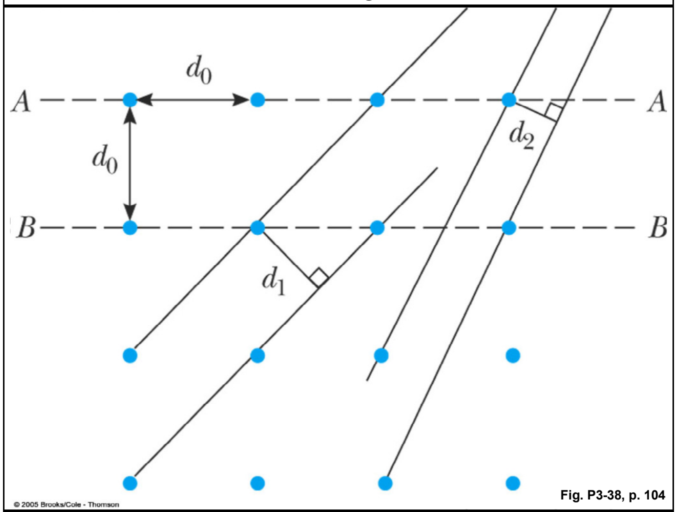
(D) X-ray photon scattered by parallel planes of a crystal



The two rays reflected by two adjacent planes have a path difference = $2d\sin\theta$
The x-ray beam is thus diffracted strongly when

$$2d\sin\theta = n\lambda \quad n = 1, 2, 3...$$

This is known as Bragg equation of diffraction.
This is the condition for observing a diffracted beam.



A sample (single phase) is characterized by
1. crystal type
2. lattice parameters: $a\ b\ c$ and angles $\alpha\ \beta\ \gamma$

For a given crystal, x-rays can be diffracted by different sets of crystal planes.

Crystal planes are labeled by Miller indices (*hkl*).
Bragg equation of diffraction due to (*hkl*) crystal planes is

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

where d_{hkl} is the interplanar spacing (≡ the perpendicular separation between parallel (*hkl*) crystal planes.
d_{hkl} can be calculated with formulae tabulated in reference book. (e.g. B.D. Cullity, *Elements of x-ray diffraction*, 2/e, QC482.D5C84 1978).