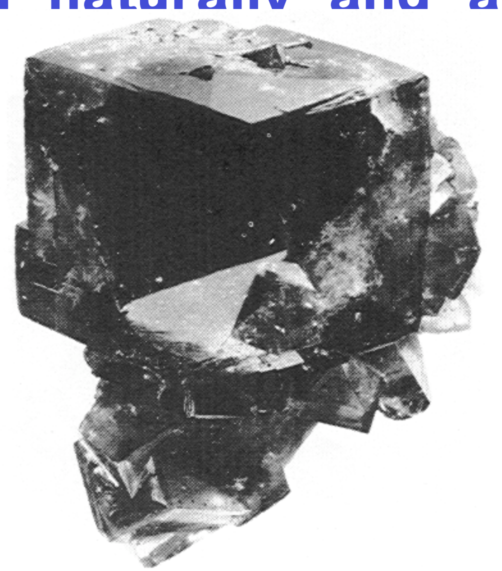
Chapter 3: Crystalline and noncrystalline materials

Outline

- Single crystals
- Polycrystalline materials
- Anisotropy
- X-ray diffraction: determination of crystal structures
- Noncrystalline solids

Single crystals

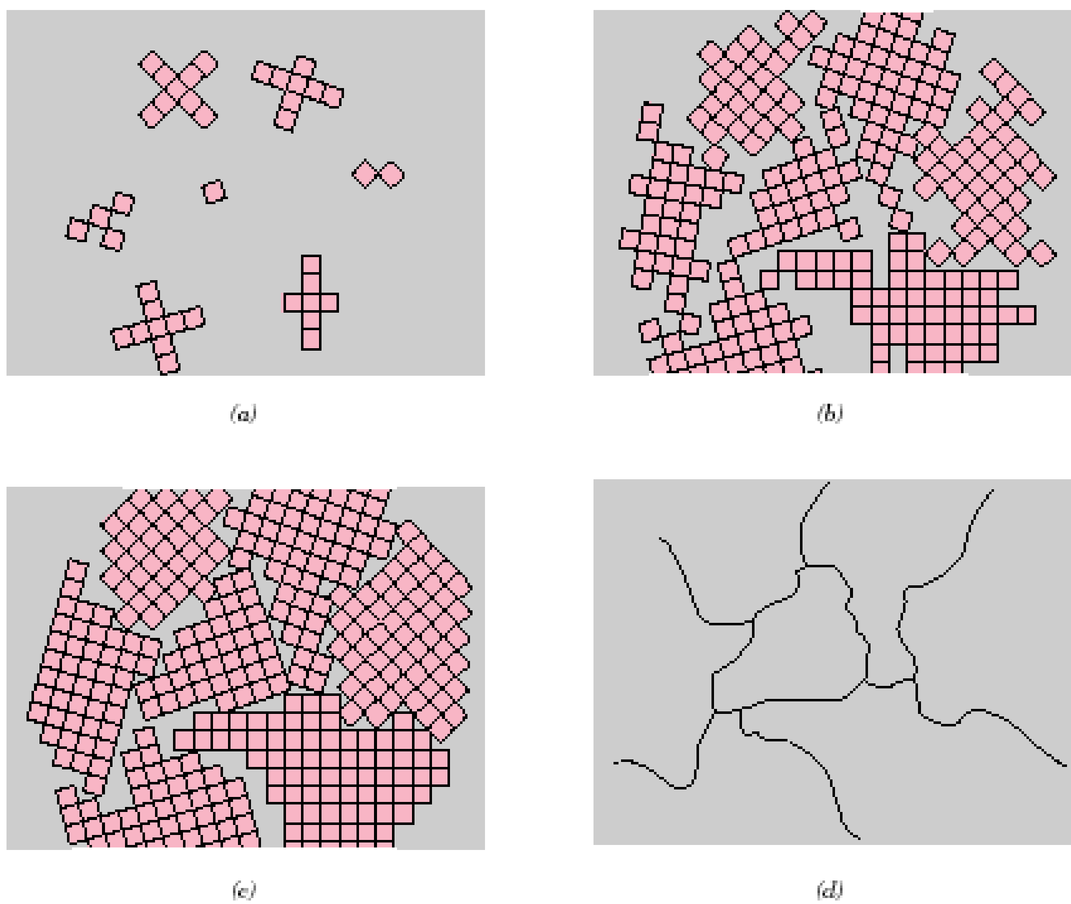
- Periodic and repeated arrangement of atoms is perfect or extends through the entirety of the specimen
- Unit cells interlock in the same way and have the same orientation
- Can be produced naturally and artificially



Single crystals of fluorite (CaF_2)

Polycrystalline materials

- A collection of many small crystals or grains
- Grain boundary: some atomic mismatch within the region where two grains meet



Anisotropy

- Anisotropy: directionality of properties
- Isotropic: properties independent of the direction of measurement

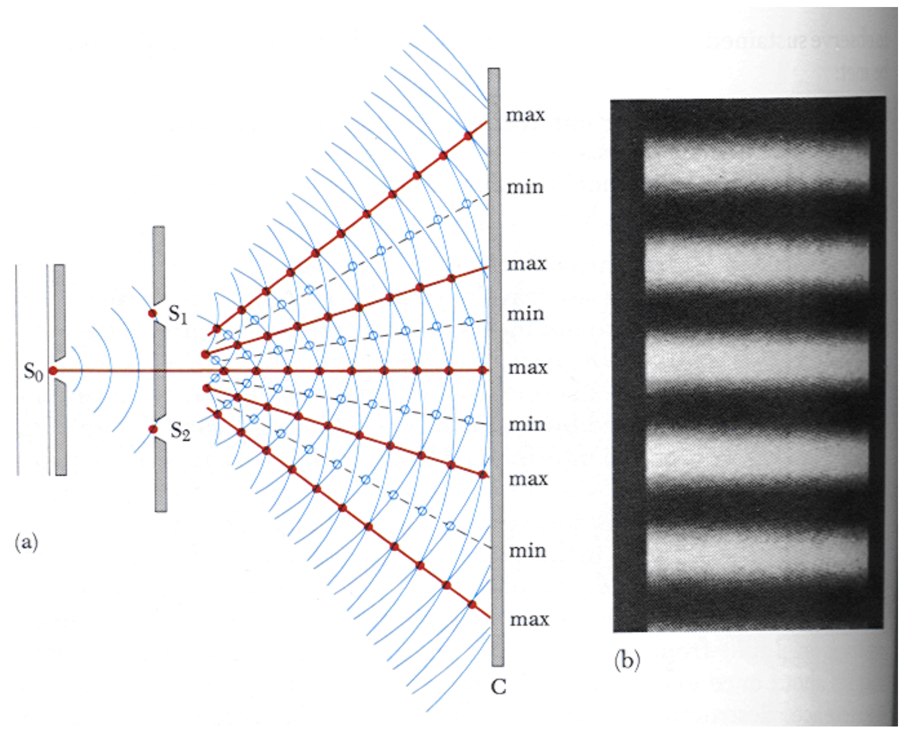
Table 3.3 **Modulus of Elasticity Values for Several Metals at Various Crystallographic Orientations**

	Modulus of Elasticity (GPa)		
Metal	[*100*]	[*110*]	[*111*]
Aluminum	63.7	72.6	76.1
Copper	66.7	130.3	191.1
Iron	125.0	210.5	272.7
Tungsten	384.6	384.6	384.6

X-ray diffraction: determination of crystal structure

❑ The diffraction phenomenon

- **Diffraction: change in the directions and intensities of a group of waves after passing by an obstacle or through an aperture**
- **Waves must be monochromatic and coherent (similar direction, amplitude**



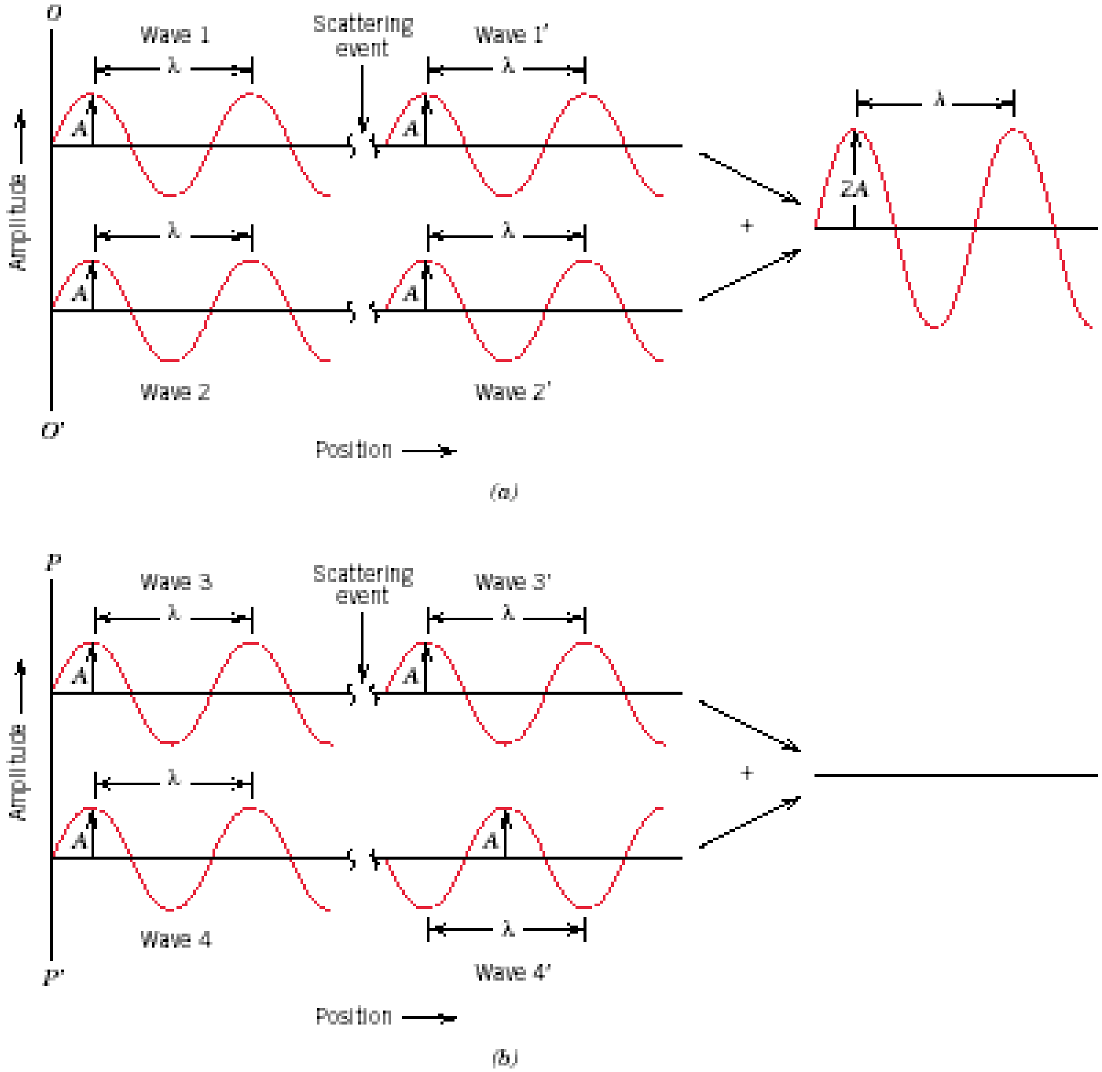
X-ray diffraction: determination of crystal structure

- **Constructive interference: the wave amplitudes are reinforced if two of the components are of the same frequency and phase (i.e. they vibrate at the same rate and are maximum at the same time)**

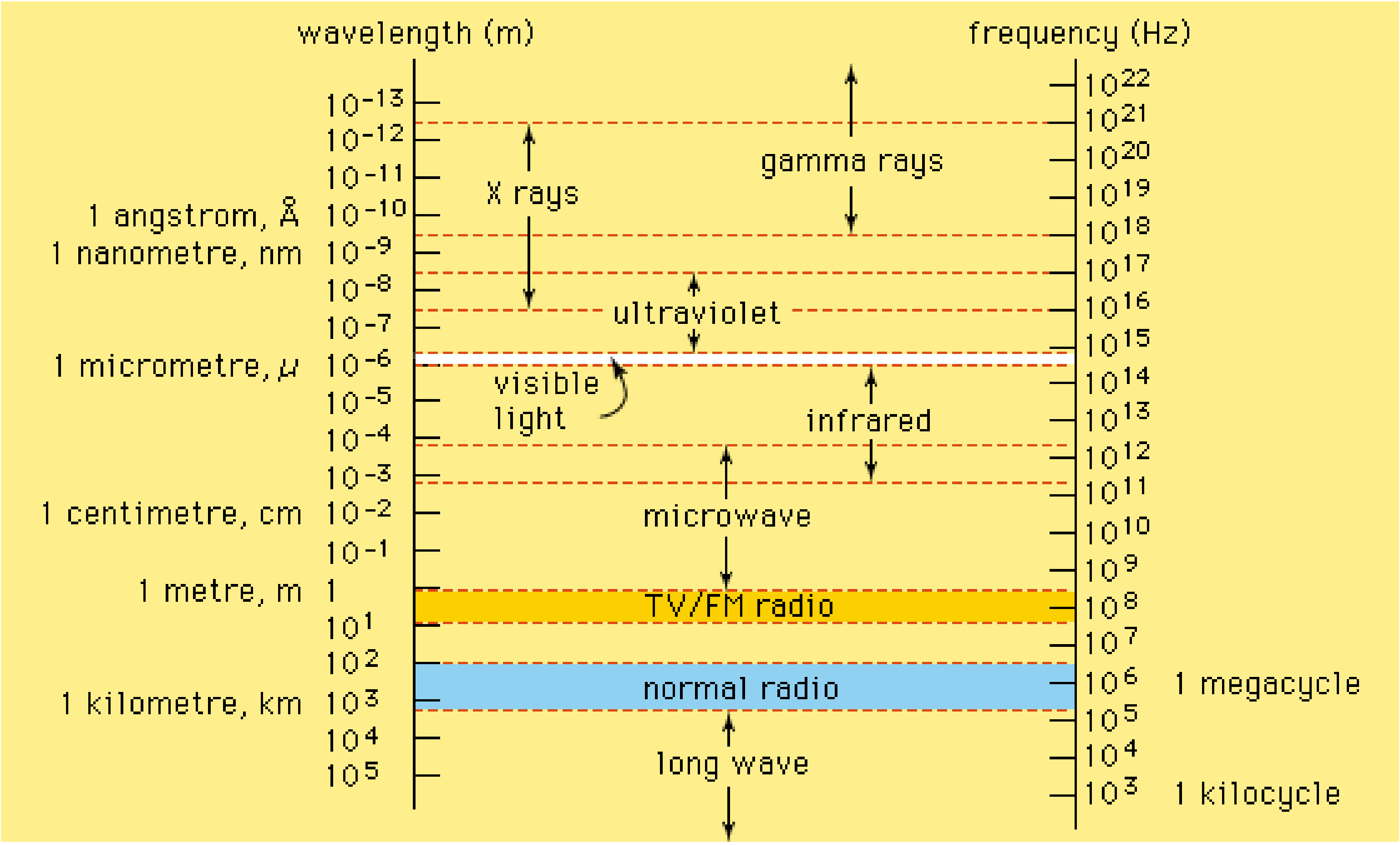
- **Destructive interference: if the two waves are out of phase by 1/2 period**

- **X-ray diffraction: a phenomenon in which the atoms of a crystal, by virtue of their uniform spacing, cause an interference pattern of the waves present in an incident beam of X rays. The atomic planes of the crystal act on the X rays in exactly the same manner as does a uniformly ruled grating on a beam of light**

X-ray diffraction: determination of crystal structure (*continue*)



The relationship of X rays to other electromagnetic radiation



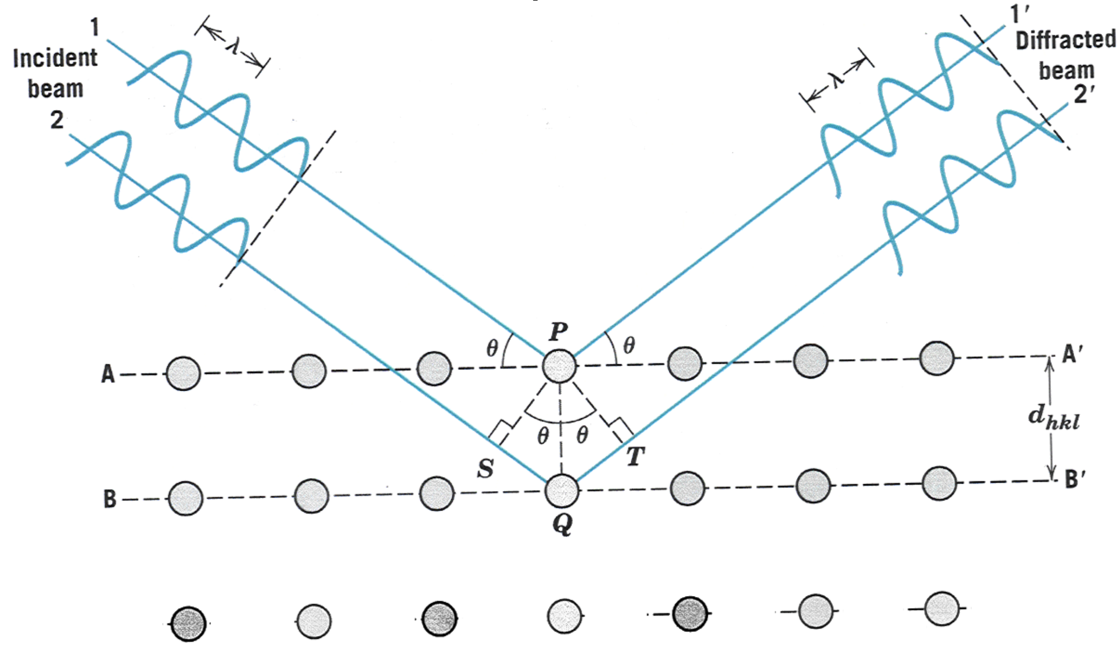
X-ray diffraction and Bragg's law

- **Bragg's law**

  Path difference $= n\lambda = d_{hkl}\sin\theta + d_{hkl}\sin\theta = 2\sin\theta$

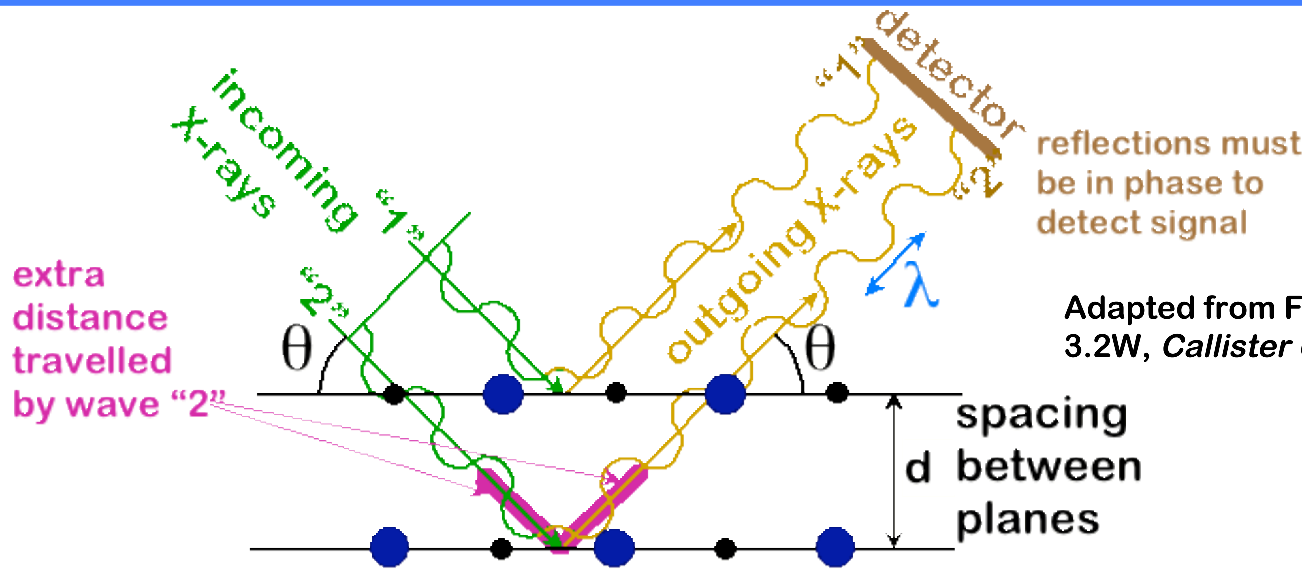
n is the reflection order and an integer; diffraction condition

- **Interplanar spacing** $d_{hkl} = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$



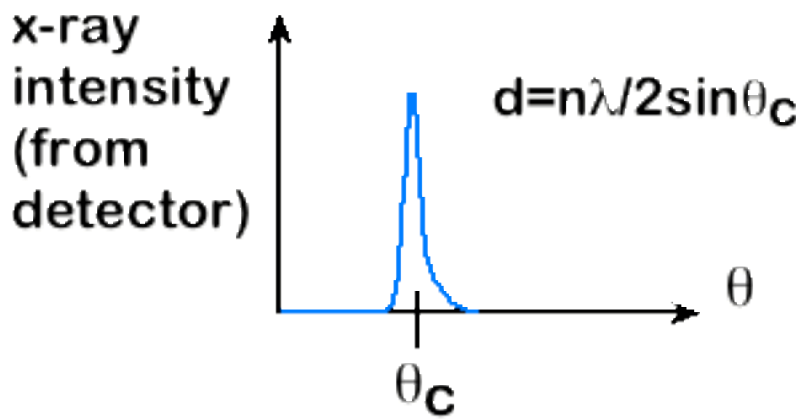
X-RAYS TO CONFIRM CRYSTAL STRUCTURE

- **Incoming X-rays diffract from crystal planes.**



Adapted from Fig. 3.2W, *Callister 6e.*

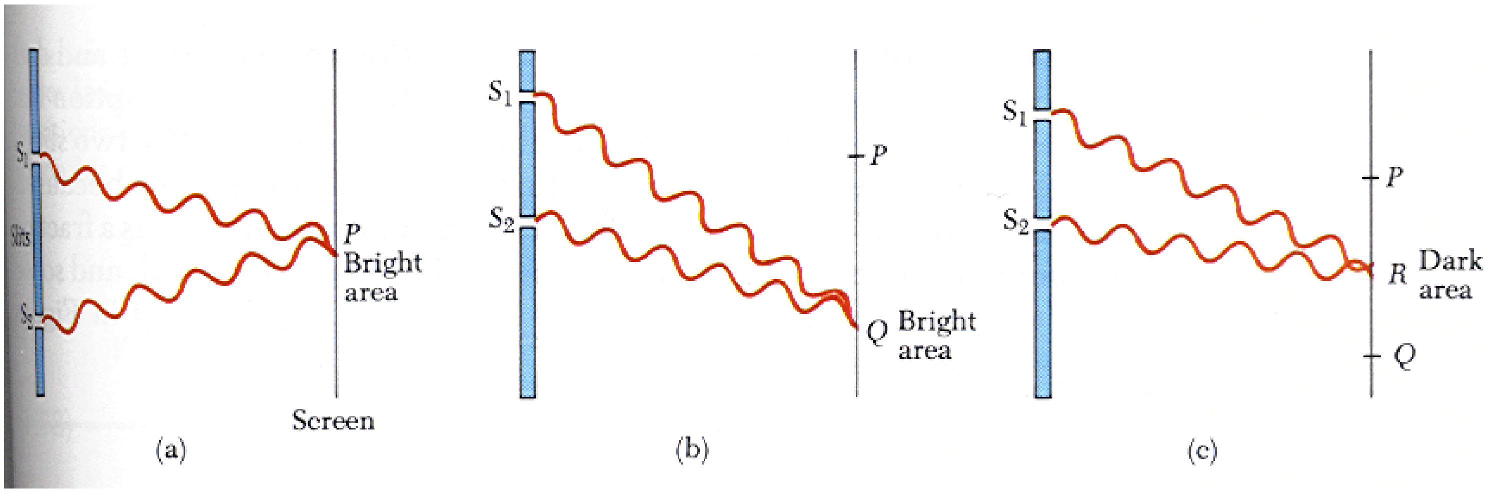
- **Measurement of:** Critical angles, θ_c, for X-rays provide atomic spacing, d.



X-ray diffraction and Bragg's law (*continue*)

- **Destructive interference**

  Path length= $\Box = (n + \frac{1}{2})\Box$
- **Bragg's law is a necessary but not sufficient condition for diffraction by real crystals**
  - **Bcc crystal structure, h+k+l must be even if diffraction is to occur**
  - **FCC crystal structure, h, k and l must all be either odd or even**



Diffraction techniques

- X-ray diffractometer

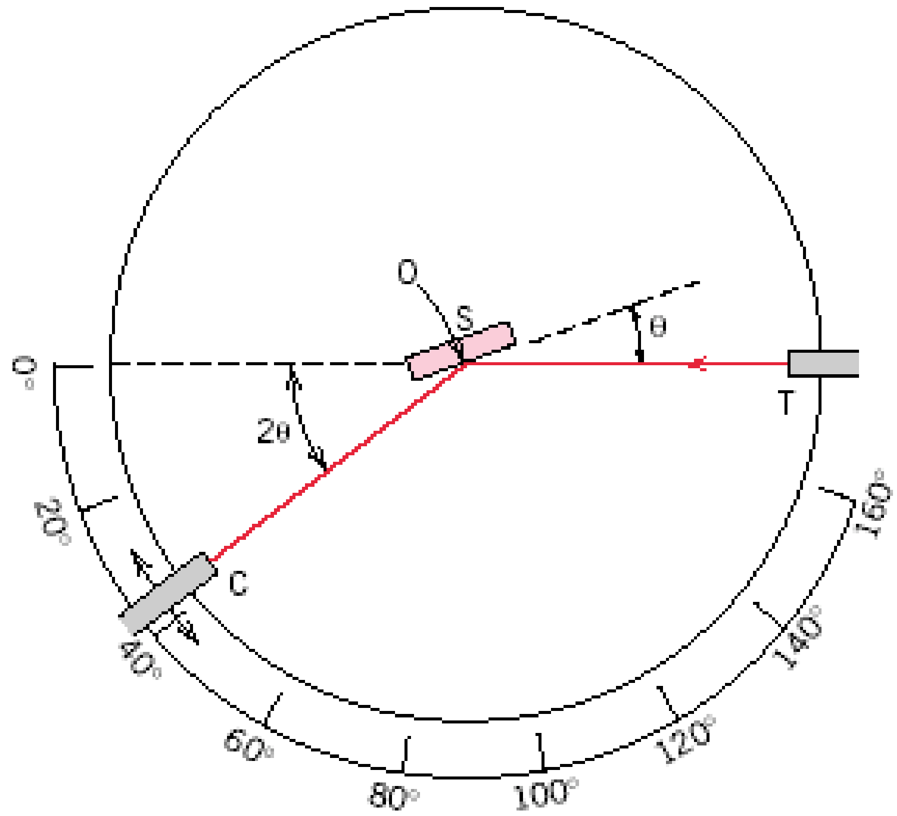


Fig 3.19 Schematic diagram of an x-ray diffractometer. T: x-ray source, S-specimen, C-detector, o-axis around which the specimen and detector rotate

Diffraction of crystals

- **Diffraction pattern for powdered lead**

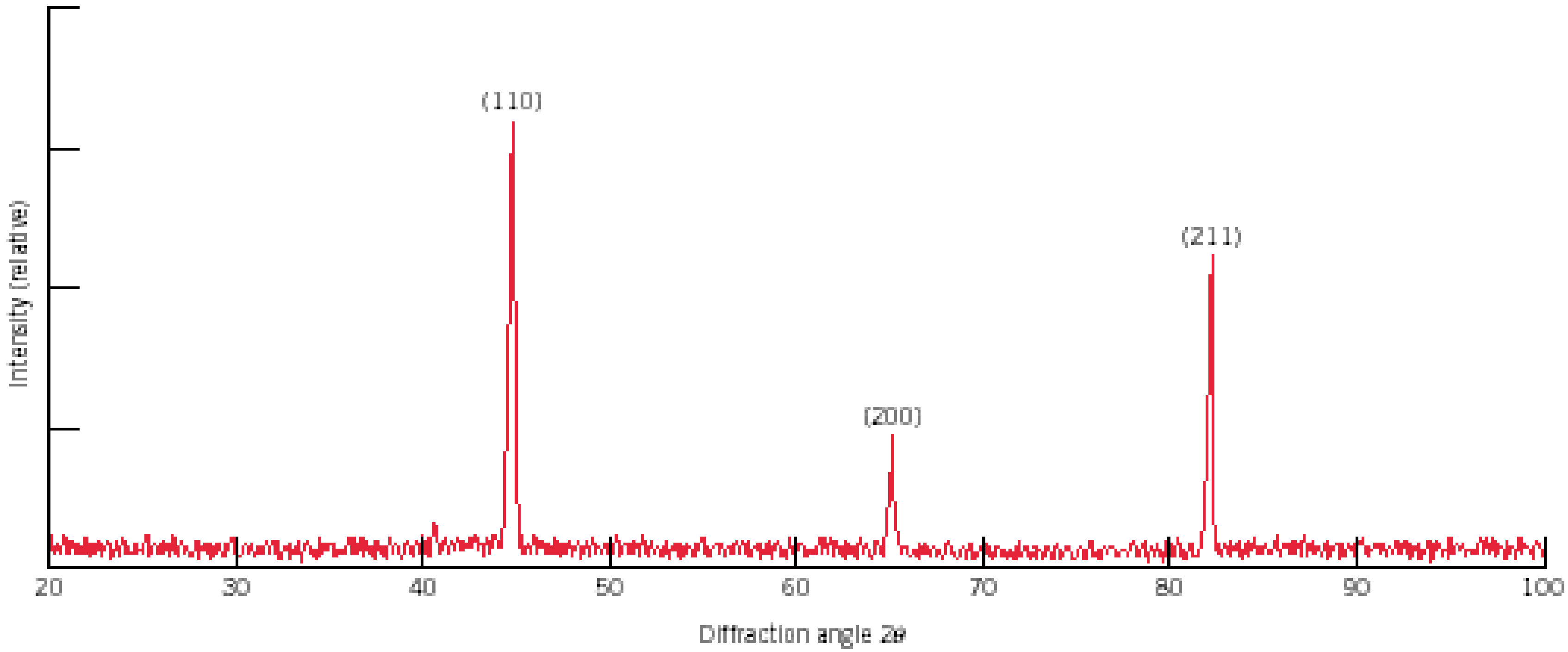


FIGURE 3.20 Diffraction pattern for polycrystalline α-iron.

Noncrystalline solids

- Noncrystalline solids: lack a systematic and regular arrangement of atoms over relatively large atomic distances (amorphous)

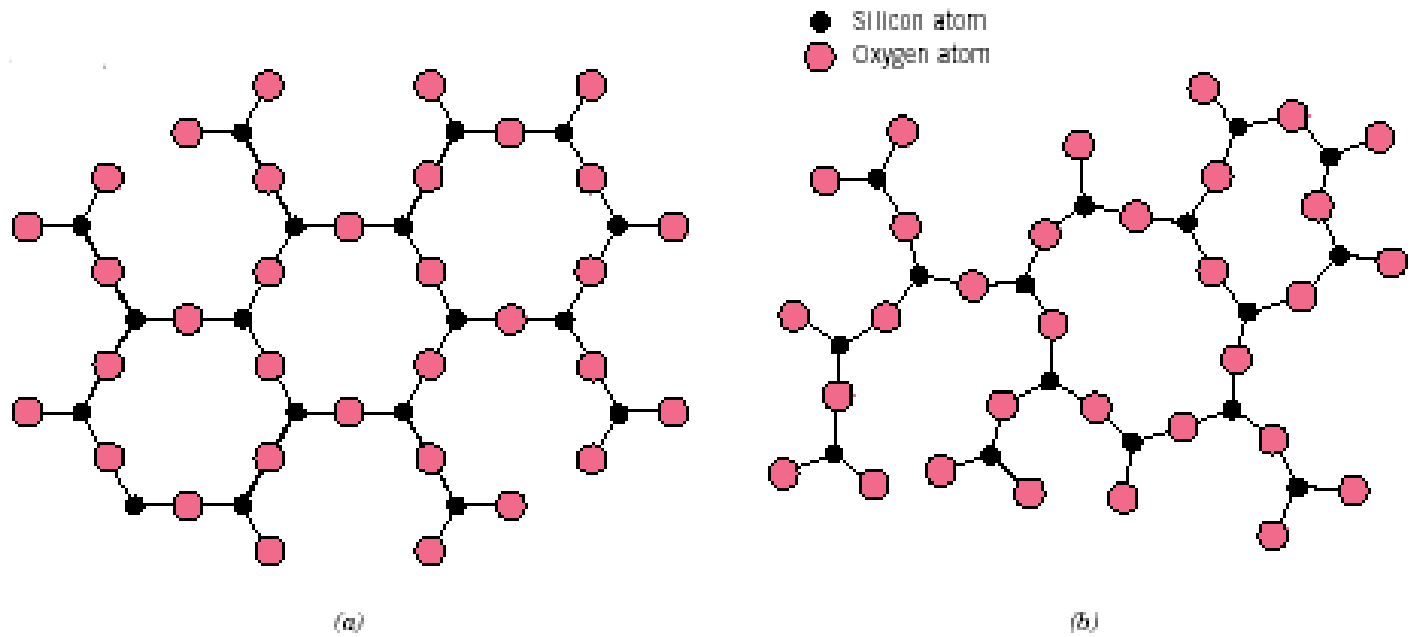


Figure 3.21 Two-dimensional schemes of the structure of (a) crystalline silicon dioxide and (b) noncrystalline silicon (b) dioxide

Calculation of diffraction angle

For BCC iron, compute (a) the interplanar spacing, and (b) the diffraction angle for the (211) set of planes. The lattice parameter for Fe is 0.2866 nm (2.866 Å). Also, assume that monochromatic radiation having a wavelength of 0.1542 nm (1.542 Å) is used, and the order of reflection is 1.

SOLUTION

(a) The value of the interplanar spacing d_{hkl} is determined using Equation 3.10, with $a = 0.2866$ nm, and $h = 2$, $k = 1$, and $l = 1$, since we are considering the (211) planes. Therefore,

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$= \frac{0.2866 \text{ nm}}{\sqrt{(2)^2 + (1)^2 + (1)^2}} = 0.1170 \text{ nm } (1.170 \text{ Å})$$

(b) The value of θ may now be computed using Equation 3.9, with $n = 1$, since this is a first-order reflection:

$$\sin\theta = \frac{n\lambda}{2d_{hkl}} = \frac{(1)(0.1542 \text{ nm})}{(2)(0.1170 \text{ nm})} = 0.659$$

$$\theta = \sin^{-1}(0.659) = 41.22°$$

The diffraction angle is 2θ, or

$$2\theta = (2)(41.22°) = 82.44°$$