

Bragg's Law

Bragg's law predicts the conditions under which diffracted x-ray beams from a crystal are possible. In deriving the law, we ignore the structure of the unit cell, which is related only to the intensities of these beams. The dashed sloping lines in Fig. 43-18a represent the intersection with the plane of the figure of an arbitrary set of planes passing through the elementary diffracting centers. The perpendicular distance between adjacent planes is d . Many other such families of planes, with different *interplanar spacings*, can be defined.

Figure 43-18b shows an incident wave striking the *family* of planes, with the incident rays making an angle θ with the plane.* For a single plane, mirror-like "reflection" occurs for *any* value of θ . To have a constructive interference in the beam diffracted from the entire family of planes in the direction θ , the rays from the separate planes must reinforce each other. This means that the path difference for rays from adjacent planes (abc in Fig. 43-18b) must be an integral number of wavelengths or

$$2d \sin \theta = m\lambda \quad m = 1, 2, 3, \dots \quad (43-12)$$

* In x-ray diffraction it is customary to specify the direction of a wave by giving the angle between the ray and the plane (the *glancing angle*) rather than the angle between the ray and the normal.

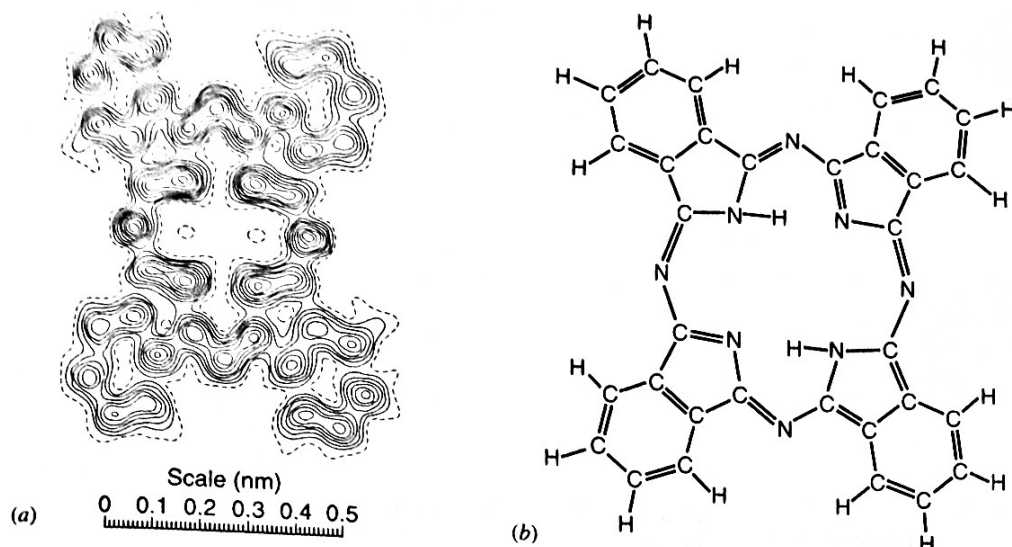


FIGURE 43-17. (a) Electron density contours for phthalocyanine ($C_{32}H_{18}N_4$) determined from the intensity distribution of scattered x rays. The dashed curves represent a density of one electron per 0.01 nm^2 , and each adjacent curve represents an increase of one electron per 0.01 nm^2 . (b) A structural representation of the molecule. Note that the greatest electron density occurs in (a) near the N atoms, which have the largest number of electrons (7). Note also that the H atoms, which contain only a single electron, are not prominent in (a).

This relation is called *Bragg's law* after W. L. Bragg, who first derived it. The quantity d in this equation (the interplanar spacing) is the perpendicular distance between the planes. For the planes of Fig. 43-18a we see that d is related

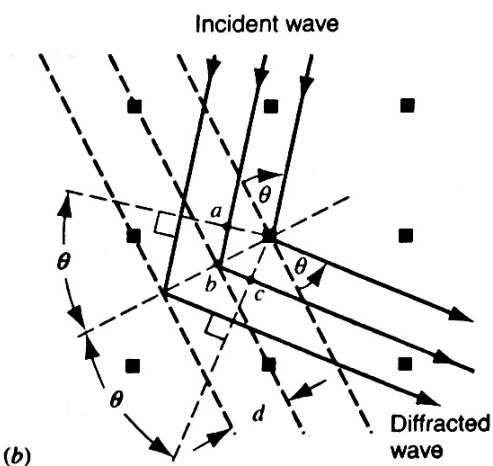
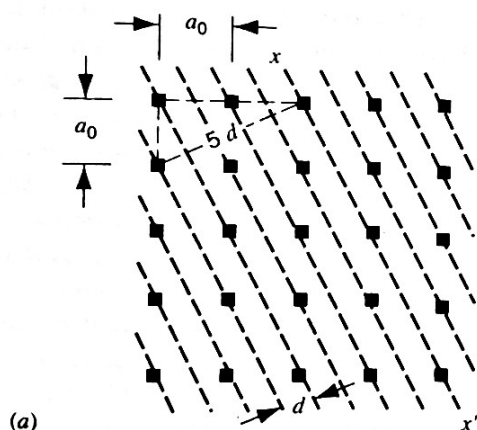


FIGURE 43-18. (a) A section through the NaCl lattice of Fig. 43-16. The dashed lines represent an arbitrary set of parallel planes connecting unit cells. The interplanar spacing is d . (b) An incident beam falls on a set of planes. A strong diffracted beam will be observed if Bragg's law is satisfied.

to the unit cell dimension a_0 by

$$d = \frac{a_0}{\sqrt{5}}. \quad (43-13)$$

If an incident monochromatic x-ray beam falls at an arbitrary angle θ on a particular set of atomic planes, a diffracted beam will *not* result because Eq. 43-12 will not, in general, be satisfied. If the incident x rays are *continuous* in wavelength, diffracted beams will result when wavelengths given by

$$\lambda = \frac{2d \sin \theta}{m} \quad m = 1, 2, 3, \dots$$

are present in the incident beam (see Eq. 43-12).

X-ray diffraction is a powerful tool for studying both x-ray spectra and the arrangement of atoms in crystals. To study the spectrum of an x-ray source, a particular set of crystal planes, having a known spacing d , is chosen. Diffraction from these planes locates different wavelengths at different angles. A detector that can discriminate one angle from another can be used to determine the wavelength of radiation reaching it. On the other hand, we can study the crystal itself, using a monochromatic x-ray beam to determine not only the spacings of various crystal planes but also the structure of the unit cell. The DNA molecule and many other equally complex structures have been mapped by x-ray diffraction methods.

SAMPLE PROBLEM 43-5. At what angles must an x-ray beam with $\lambda = 0.110 \text{ nm}$ fall on the family of planes represented in Fig. 43-18b if a diffracted beam is to exist? Assume the material to be sodium chloride ($a_0 = 0.563 \text{ nm}$).

Solution The interplanar spacing d for these planes is given by Eq. 43-13, or

$$d = \frac{a_0}{\sqrt{5}} = \frac{0.563 \text{ nm}}{\sqrt{5}} = 0.252 \text{ nm}.$$

Equation 43-12 gives

$$\theta = \sin^{-1} \left(\frac{m\lambda}{2d} \right) = \sin^{-1} \left(\frac{(m)(0.110 \text{ nm})}{(2)(0.252 \text{ nm})} \right).$$