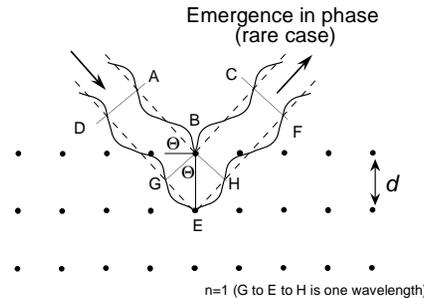
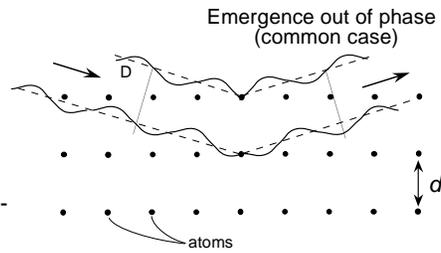


## X-ray Diffraction and the Powder Method

As X-rays pass through a crystal, they strike individual atoms and transfer energy to those atoms. That energy is re-radiated away at the same wavelength. Most such re-radiated energy is out of phase and so interferes destructively, so that it's not detectable (upper case at right). However, certain geometries allow the newly generated X-rays to emerge in phase, or to constructively interfere, to produce detectable X-radiation (lower case at right). Such a geometry requires that the spacing between planes of atoms,  $d$ , allow  $n$  to be an integer in Bragg's Law.



Mathematically:

$$GE + EH = n\lambda \quad GE = EH$$

$$GE = \frac{n\lambda}{2} \quad \sin\theta = \frac{GE}{d} \quad \text{from geometry at right}$$

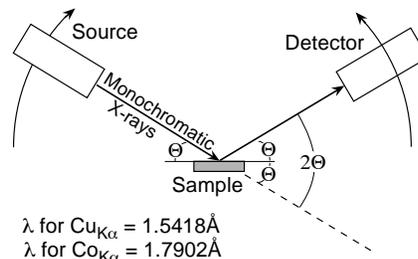
$$\sin\theta = \frac{\frac{n\lambda}{2}}{d} \quad \text{by substitution}$$

Bragg's Law:

$$n\lambda = 2d\sin\theta \quad \text{by algebraic rearrangement}$$

The geometry at right would allow us to determine the distance  $d$  (the distance between planes of atoms) if we rotated an X-ray source and an X-ray detector through all possible values of  $\theta$ . That's what an X-ray diffractometer does. The source is a metal that is bombarded with electrons to cause displacement of inner-shell electrons, and thus emission of X-rays, as electrons return to K shells (thus, for example,  $\text{Cu}_{K\alpha}$  or  $\text{Co}_{K\alpha}$  radiation). That source is swung through  $\theta = \sim 1^\circ$  to  $\theta = \sim 35^\circ$ , or through a smaller range as desired. At the same time, the

X-ray Diffractometer:

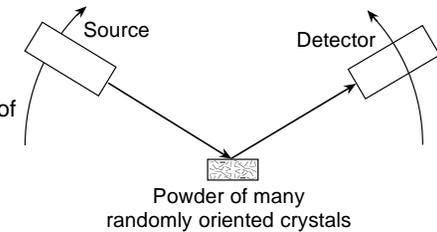
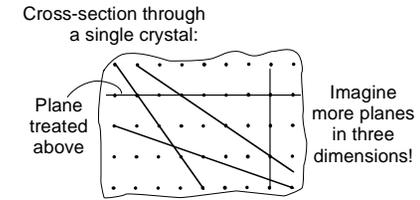


$\lambda$  for  $\text{Cu}_{K\alpha} = 1.5418\text{\AA}$   
 $\lambda$  for  $\text{Co}_{K\alpha} = 1.7902\text{\AA}$

detector is swung through the same range of  $\theta$  on the other side. Alternately, the source is fixed, the sample rotates, and detector moves at an angular rate twice that of the sample. The angle made by the

source, sample, and detector is thus  $2\theta$ , the parameter reported on plots of measured intensity of diffracted X-rays.

As we've imagined X-ray diffraction thus far, we would only be able to measure one  $d$ -spacing (the distance between planes of one parallel set). To measure all other possible  $d$ -spacings (see sketch at right), we would need to rotate the crystal through all possible orientations. Instead, the Powder Method uses a pulverized sample in which thousands of small crystals are (hopefully) randomly oriented so that one sweep of source and detector causes diffraction on all possible crystallographic planes and thus produces all possible peaks on the diffractogram.



The point of all this is that

We can identify minerals by their unique combinations of  $d$ -spacings and peak heights (by comparing the diffractogram of an unknown mineral with databases compiled for all known minerals), and

We can characterize the ordering, size of domains, and minor element chemistry of minerals from the shapes and positions of peaks.

