Chapter 3: Structures via Diffraction

Goals

– Define basic ideas of diffraction (using x-ray, electrons, or neutrons, which, although they are particles, they can behave as waves) and show how to determine:

- Crystal Structure
- Miller Index Planes and Determine the Structure
- Identify cell symmetry.

Chapter 3: Diffraction

Learning Objective

Know and utilize the results of diffraction pattern to get:

– lattice constant.

– allow computation of densities for close-packed structures.

– Identify Symmetry of Cells.

– Specify directions and planes for crystals and be able to relate to characterization experiments.

CRYSTALS AS BUILDING BLOCKS

- ***Some*** **engineering applications require single crystals:**

--diamond single crystals for abrasives

(Courtesy Martin Deakins, GE Superabrasives, Worthington, OH. Used with permission.)

--turbine blades

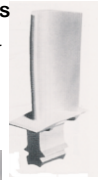


Fig. 8.30(c), *Callister 6e.* (Fig. 8.30(c) courtesy of Pratt and Whitney).

- **Crystal properties reveal features of atomic structure.**

--Ex: Certain crystal planes in quartz fracture more easily than others.

(Courtesy P.M. Anderson)

POLYCRYSTALS

- ***Most*** **engineering materials are polycrystals.**

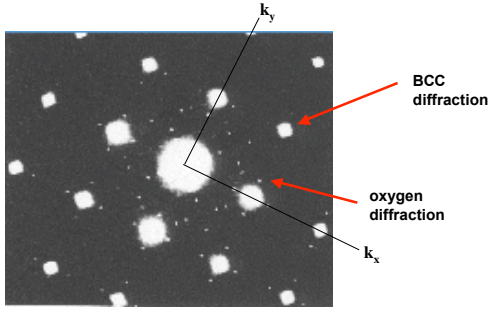
Adapted from Fig. K, color inset pages of *Callister 6e.* (Fig. K is courtesy of Paul E. Danielson, Teledyne Wah Chang Albany)

Nb-Hf-W plate with an electron beam weld.

- **Each "grain" is a single crystal.**
- **If crystals are randomly oriented, overall component properties are not directional.**
- **Crystal sizes range from 1 nm to 2 cm (i.e., from a few to millions of atomic layers).**

SIMPLE Diffraction in Crystals and Polycrystals

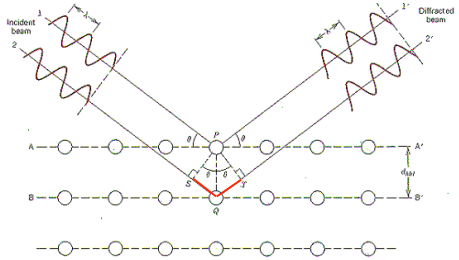
Diffraction Pattern Transmission Electron Microscopy (TEM)
Tantalum with BCC ordered structure containing Oxygen.



Two ordered patterns appear, one w/ Ta and the other w/ O.

Diffraction by Planes of Atoms

Light gets scattered off atoms…But since *d* (atomic spacing) is on the order of angstroms, you need **x-ray diffraction** (wavelength ~ d).



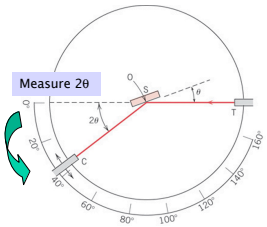
To have constructive interference (I.e., waves ADD).

$$n\lambda = \bar{SQ} + \bar{QT}$$

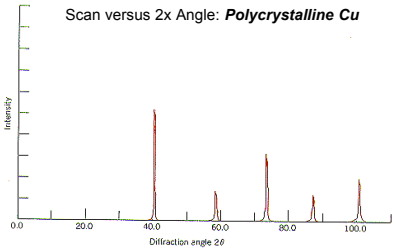
$$n\lambda = d_{hkl}\sin\theta + d_{hkl}\sin\theta = 2d_{hkl}\sin\theta$$

Diffraction Experiment and Signal

Diffraction Experiment



Scan versus 2x Angle: ***Polycrystalline Cu***



Diffraction collects data in "***reciprocal space***" since it is the equivalent of a ***Fourier transform of "real space***", i.e., e^{ikr}, as k ~ 1/r.

How can 2θ scans help us determine crystal structure type and distances between Miller Indexed planes (I.e. structural parameters)?

Crystal Structure and Planar Distances

Bravais Lattice	Constructive Interference	Destructive Interference
	Reflections present	Reflections absent
BCC	(h + k + l) = Even	(h + k + l) = Odd
FCC	(h,k,l) All Odd or All Even	(h,k,l) Not All Odd or All Even
HCP	Any other (h,k,l)	h+2k=3n, l = Odd n= integer

h, k, l are the Miller Indices of the planes of atoms that scatter!

So they determine the important planes of atoms, or symmetry.

Distances between Miller Indexed planes

For cubic crystals:

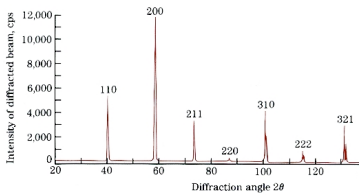
$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

For hexagonal crystals:

$$d_{hkl} = \frac{a}{\sqrt{\frac{4}{3}(h^2 + hk + k^2) + l^2\left(\frac{a}{c}\right)^2}}$$

Allowed (hkl) in FCC and BCC for principal scattering (n=1)

Self-Assessment:
From what crystal structure is this?



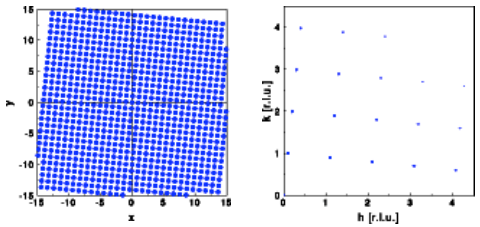
(h k l)	$h^2+k^2+l^2$	h+k+l	h,k,l all even or odd?
100	1	1	No
110	2	**2**	No
111	3	3	Yes
200	4	**2**	Yes
210	5	3	No
211	6	**4**	No
220	8	**4**	Yes
221	9	5	No
300	9	3	No
310	10	**4**	No
311	11	5	Yes
222	12	**6**	Yes
320	13	5	No
321	14	**6**	No

h + k + l was even and gave the labels on graph above, so crystal is BCC.

Diffraction of Single 2D Crystal Grain

Lattice of Atoms: Crystal Grain

Diffraction Pattern in (h,k) plane



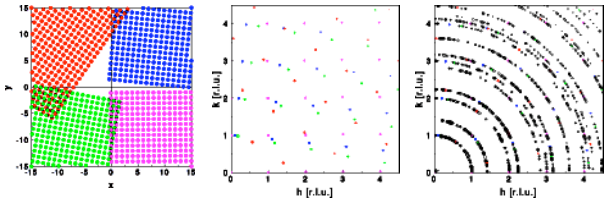
Powder diffraction figures taken from Th. Proffe and R.B. Neder (2001)
http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/pow_a.html

Diffraction of Multiple Single 2D Crystal Grains (powders)

Multiple Crystal Grains:
4 Polycrystals

Diffraction Pattern
in (h,k) plane (4 grains)

Diffraction Pattern
in (h,k) plane (40 grains)



Powder diffraction figures taken from Th. Proffe and R.B. Neder (2001)
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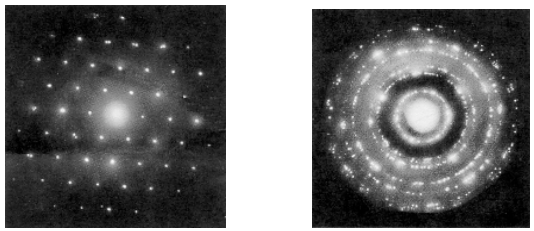
Example from Graphite

Diffraction from Single Crystal Grain

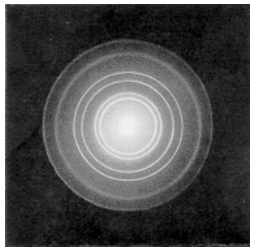
Mutlple Grains: Polycrystal



Powder diffraction figures taken from Th. Proffe and R.B. Neder (2001)
http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/pow_a.html

Example from Aluminum

Diffraction from Mutlple Grains of Polycrystalline Aluminum



Powder diffraction figures taken from Th. Proffe and R.B. Neder (2001)

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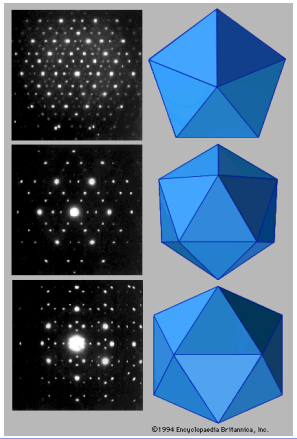
Example from QuasiCrystals

Remember there is no 5-fold symmetry alone that can fill all 3-D Space!



SUMMARY

• Materials come in **Crystalline** and **Non-crystalline** Solids, as well as **Liquids/Amoprhous**. Polycrystals are important.

•Crystal Structure can be defined by space lattice and basis atoms (lattice decorations or motifs), which can be found by diffraction.

• Only 14 Bravais Lattices are possible (e.g. FCC, HCP, and BCC).

• Crystal types themselves can be described by their atomic positions, planes and their atomic packing (linear, planar, and volumetric).

• *We now know how to determine structure mathematically and experimentally* by diffraction.