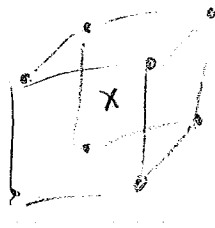


003 3 1.

Cesium Chloride - like bcc, but diff atom in middle

bring computer  
+ show  
structure



$\circ = \text{Cs}^+$   
 $\times = \text{Cl}^-$

How many  $\text{Cl}^-$  ions for each  $\text{Cs}^+$  ion? (Just 1)

WKL

what is lattice?

sc

basis:  $\text{Cs}^+$  at  $(0,0,0)$   
 $\text{Cl}^-$  at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

CsCl structure used by

BeCu  
AlNi  
CuZn ("brass")  
CuPd  
AgMg

LiHf  
NH<sub>4</sub>Cl (?)  
TiBr  
(CsCl)  
TiI

1:1 stoichiometry

Question: do compounds with just one element have to have 1 atom in unit cell?

→ No! Ex: bcc, fcc already discussed.

OK, that's "cheating" because primitive unit cells for bcc, fcc have only 1 atom in them.

→ still No! Next structure (hcp) is an example.

HCP hexagonal close packed

★ fig 19 pg 15

Arrangement ABAB = "hcp"  
 ABCABC = fcc, surprisingly  
 empty (filled at angles)

(Note dense elements  
 Pt, Au, Pb  
 are all fcc)

both are "close packed",  
 maximizing packing fraction,  
 % of space filled w/ spheres  
 = 74%

lattice = hexagonal  
 2 atoms/unit cell

★ Fig 21 pg 16

if not close-packed, still related. Just diff. % atoms

block list:	Hg	Zn	Zr
	Isa	Cd	Gd
	Mg	Co	Lu
	Ti	Y	

Need to fully understand differences between

lattice and structure

only the case of 1 atom/unit cell.  
 (as obviously one type of atom only)

In general they are very different

Diamond structure

- tetrahedral bonds

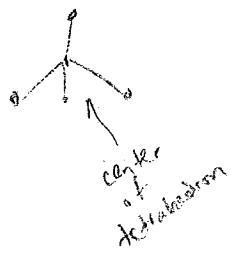


Fig 23 pg 17

lattice? fcc

2 atoms in basis  $\begin{pmatrix} 000 \\ \frac{1}{4} \frac{1}{4} \frac{1}{4} \end{pmatrix}$

8 atoms in "conventional" unit cell  
(8 atom basis listed in book)

relatively empty:

34% packing fraction  
(less than  $\frac{1}{2}$  of hcp or fcc)

Why? covalent bonding  
4 valence electrons

Elements

- Carbon (diamond)
- silicon
- germanium
- tin

"Zincblende"

ZnS structure

Fig 24 pg 18

- exactly like diamond, but 2 types of atoms



1:1 stoichiometry

fcc still

basis atom A  $000$   
B  $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

crystals

- |       |      |
|-------|------|
| SiC   | ZnSe |
| (ZnS) | GaAs |
| AlP   | AlAs |
| GeP   | InSb |

last comments on Ch 1

1) Lowest energy structure depends on Temp + pressure

Ex: apply enough P, can get almost anything to switch to close-packed

(→ Gus Hart's research)

So don't take my info as gospel

2) Table 4 p 21

a) density vs atomic concentration  
 $\frac{g}{cm^3}$  vs  $\frac{\# \text{ atoms}}{cm^3}$

b) nearest neighbor - a few angstroms  $\lambda$   
 $1 \text{ nm} = 10 \text{ \AA}$

3) Not mentioned is Kittel

There are an infinite number of crystals that could be formed (because eg. the basis atoms could be located at any real numbers).

However, there are not an infinite number of ways of classifying the crystals by symmetry. (rotations, translations, etc.)

There are 230 distinct "space groups" (of which the Bravais lattices are 14) (and diamond, zincblende, hcp are 3 others)

They are usually divided into 32 "crystal classes" (categories)

(sc, fcc, bcc, diamond all in same crystal class, but in diff space groups)

which share "point group symmetries" (rotation, reflection, inversion, mirror, as previously mentioned)

Chapter 2

Diffraction - (waves by crystals)

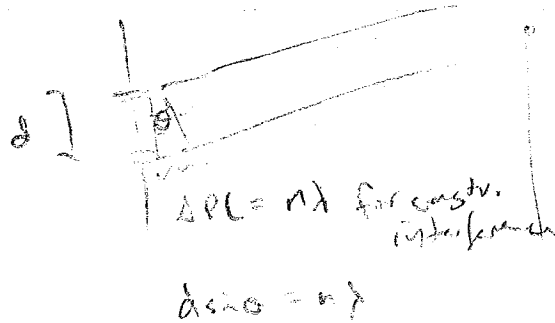
bring computer to show Stokes demo

How do we know the structure? Density of atoms

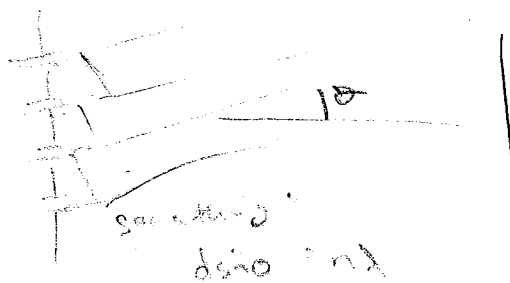
But angles: every direction different

$\lambda \approx \text{a few } \text{\AA}$  angles such that  $d \sin \theta \approx \text{a few } \text{\AA}$

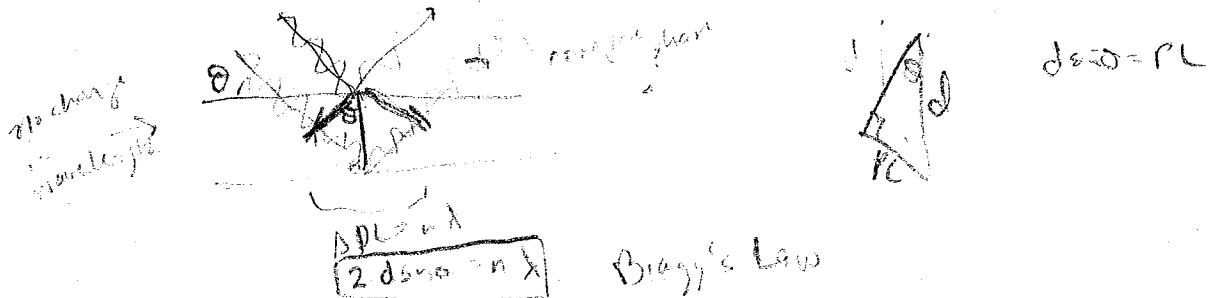
Diffraction by doublet (pages 23)



Diffraction by gratings (page 23)



Diffraction by planes (maxima/minima not 23)



Note: this occurs reflection is specular. Why is that?

\* Slides reflection from planes