Prog 1

Some real materials! (1...Prog)

Elements pg 20 ✱

✱ bcc: Li, Na, K, V, Cr, Fe, Rb, Nb, Mo, Cs, Ba, Ta, W, Eu

✱ fcc: Ne, Al, Ar, Ca, Ni, Cu, Kr, Sr, Rh, Pd, Ag, Xe, Ir, Pt, Au, Pb, Ac, Ce, Yb, Th

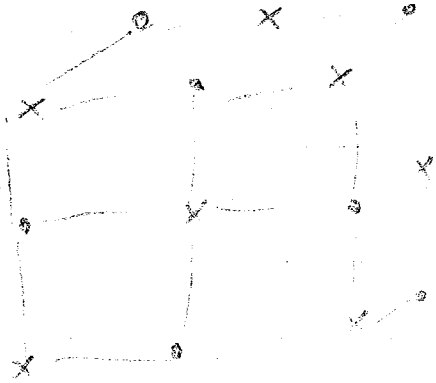
✱ hcp

maybe diamond because of 2 elements

http://cst-www.nrl.navy.mil/lattice

also Stble's website

Sodium chloride



Lattice = ? fcc, not sc

basis: Cl^- in at 000
Na^+ in at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

8 atoms in conventional unit cell

"NaCl structure" = name of this structure ✱, also used by other crystals

book list:

(LiH)	AgBr
MgO	PbS
MnO	KCl
(NaCl)	KBr

Note 1:1 stoichiometry

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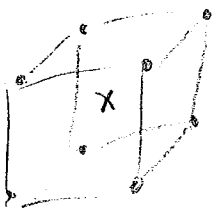
Cesium Chloride – like bcc, but diff atom in middle



o = Cs^+
x = Cl^-

How many Cl^- ions for each Cs^+ ion? (Just 1)

Wrong

what is lattice? sc

basis: Cs^+ at 000
Cl^- at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

CsCl structure used by

BeCu	LiHg
AlNi	NH_4Cl (?)
CuZn ("β-brass")	TlBr
CuPd	(CsCl)
AgMg	TlI

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.

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HCP hexagonal close packed

★ fig 19 pg 15

Arrangement ABAB = "hcp"
ABCABC = fcc, surprisingly enough (filled at an angle)

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

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

lattice = hexagonal
2 atoms/unit cell

Fig 21 pg 16 ★

almost close-packed, still related. Just diff. c/a ratio

book list:

He	Zn	Zr
Be	Cd	Gd
Mg	Co	Lu
Ti	Y	

Need to fully understand difference between

lattice and structure

only the case if 1 atom / (unit) cell
(and obviously one type of atom only)

In general they are very different

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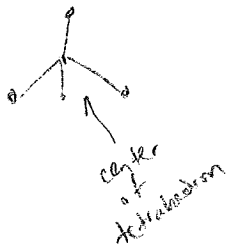
day 3 of 4

Diamond structure

- tetrahedral bonds

Fig 23 of 17



lattice? fcc

2 atoms in basis 000
¼ ¼ ¼

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

relatively empty:
34% packing fraction
(less than ½ of hcp + fcc)

Why? covalent bonding
4 valence electrons

Elements
carbon (diamond)
silicon
germanium
tin

"Zincblende"
ZnS structure

Fig 24 of 18

- exactly like diamond, but 2 types of atoms

fcc still

basis atom A 000
B ¼ ¼ ¼

1:1 stoichiometry

Crystals

SiC	ZnSe
(ZnS)	GaAs
AlP	AlAs
GaP	InSb

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Last comments on Ch 1

1) Lowest energy structure depends on Temp + pressure

Ex: apply enough press, can get almost anything to structure to close-packed

(→ Gus Hart's research)

So don't take my info as gospel

2) Table 4 pg 21

a) density vs atomic concentration

$\frac{g}{cm^3}$ $\frac{\#\ atoms}{cm^3}$

b) nearest neighbor - a few angstrom Å

1 nm = 10 Å

3) Not mentioned in Kittel

There are an infinite number of crystals that could be formed (because e.g. 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) which share "pt group symmetries" (rotation, reflection, inversion, combo, as previously mentioned)

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

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