Caesium Chloride - like bcc, but different mode

$\text{Ca}^+ \quad \text{Cl}^-$

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

What is lattice? $\text{Se}$

\[ \text{basis: } \text{Ca}^+ \text{ at } 0.00 \text{, Cl}^- \text{ at } \frac{1}{2} \frac{1}{2} \frac{1}{2} \]

CaCl$_2$ structure used by

\begin{align*}
\text{BeCu} & \\
\text{AlNi} & \\
\text{CuZn (\text{g.p.m.})} & \\
\text{CuPb} & \\
\text{AgMg} & \\
\end{align*}

\begin{align*}
\text{LiH} & \\
\text{NH}_4\text{Cl (\text{?})} & \\
\text{TiBr} & \\
\text{CsCl (\text{?})} & \\
\text{I} & \\
\end{align*}

Lif which model

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

\[ \text{No!} \] Ex: bcc, as already discussed.

Ok, that's "cloaking", because you have unit cells forebce fece have only 1 atom in them.

\[ \text{Still no! Next section (hex) is an example.} \]
HCP  
Hexagonal close-packed

\[ \text{Fig 19, p. 15} \]

Arrangement: ABAAB = "hep"
ABCABC = "fcc",

surprisingly,

(No. 37) or (37)  
(No. 15) or (15)

(NOTE: Some elements
Pt, Au, Pb
are all FCC)

lattice = hexagonal

2 layers/unit cell

\[ \text{Fig 21, p. 16} \]

fcc close-packed, still related. Just differ $\frac{\sqrt{3}}{2}$ a radians

bulk list:  
H,  
Zn,  
Cd,  
Mg,  
Ca,  
Y

Need to fully understand difference between

\underline{lattice} \quad \underline{and} \quad \underline{structure}

only two cases of 1 atom/unit cell.

(In reality more types of atoms may)

In general they are very different.
**Diamond Structure**

- tetrahedral bonds

![Fig 23 @ 17](image)

(enamel)

- carbon (diamond)
- silicon
- germanium
- Si

8 atoms in "conventional" unit cell

- 8 atoms in "conventional" unit cell

-face centered cubic:

- 34.7% packing fraction
- (less than 2/3 of hcp stack)

 WHY? covalent bonding

- 4 valence electrons

**Zincblende**

- 2 atoms

![Fig 24 @ 1B](image)

- exactly like diamond, but 2 types of atoms

FCC still

- basis: atom A: 000
- B: 1/2 1/2 1/2

1:1 stoichiometry

**Crystals**

- SiC
- ZnSe
- InSb
- AlP
- GaP
- InP
- GaAs
- AlAs
last comments on Ch 1

1) Lowest energy structure depends on Temp + pressure

Ex: silver enough time, can get almost anything to solidify + close-packed

(BO Gus Heri's argument)

So don't take my info as gospel

2) Table 4 pg 21

a) density vs atomic concentration

\[ \text{density} \quad \frac{\text{atoms}}{\text{cm}^3} \]

b) nearest neighbor - a few angstroms

1 nm = 0.1 \AA

3) Not mentioned in lecture

There are an infinite number of crystals that can be formed (because, e.g., the basis atoms can be located at any 3-D repeat).

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

There are 230 distinct "space groups" (of which the usual lattice is 1/1)

(normal, orthorhombic, hexagonal, cubic, etc.)

They are usually divided into 32 "crystal classes" (point groups)

(sc, tet, hex, diamond, etc.) which share "primitive symmetries" (rotation, reflection, inversion, etc.)

Carb, e.g. mainly monoclinic
Chapter 2

Diffraction by Crystals

1. How do we know the structures? Peierls Approximation

2. van der Waals interaction + dispersion

\[ \lambda \approx a \]  \hspace{1cm} \text{where} \ a \approx \text{a few Å}

Diffraction by Doubly (Page 163)

\[ d \]

\[ \theta \]

\[ \Delta L = n\lambda \] for constructive interference

\[ d \sin \theta = n\lambda \]

Diffraction by Grading (Page 167)

\[ d \]

\[ \theta \]

\[ \sin \theta = n\lambda \]

Diffraction by Planes (Page 164)

\[ d \]

\[ \theta \]

\[ \Delta l = n\lambda \]  \hspace{1cm} \text{Bragg's Law}

Note: this could occur in reflection + specular Bragg's Law

\[ \frac{1}{d} \Delta \theta = n\lambda \]

\[ \text{Slated reflection from plane } \]