

Coordination Number

the number of nearest neighbors

simple cubic 6

bcc 8

fcc 12

Wigner-Seitz Primitive Cell

This is a construction to determine a special primitive cell and can be performed in 2-D or in 3-D.

1. start from a given lattice point
2. define vectors to each nearest neighbor (+ 2nd, 3rd, etc)
3. bisect the vector with a line or plane \perp to the vector at the midpoint
4. the area or volume so bounded by lines or planes will be the Wigner-Seitz primitive unit cell.

Nice feature is that the Wigner-Seitz unit cell has the same symmetry as the lattice itself.

Study: carefully consider the formation of Wigner-Seitz primitive cells for

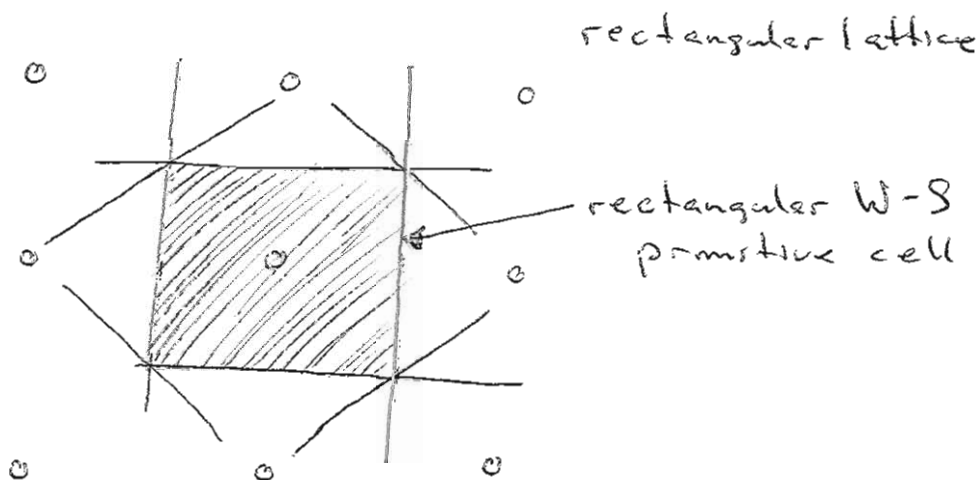
- sc
- bcc
- fcc

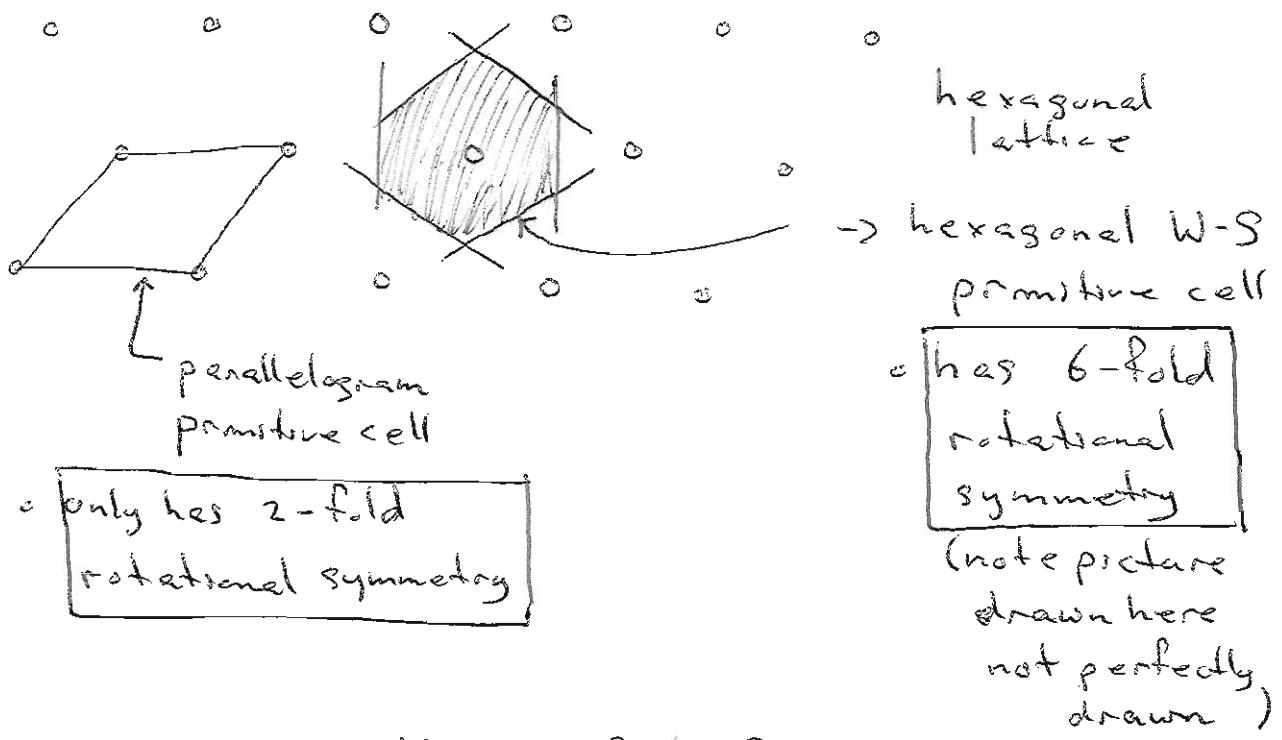
compare the Wigner-Seitz primitive cells with the primitive cells obtained using the parallelepiped method

how are they different?

what do they have in common?

Wigner-Seitz cell in 2-D: example

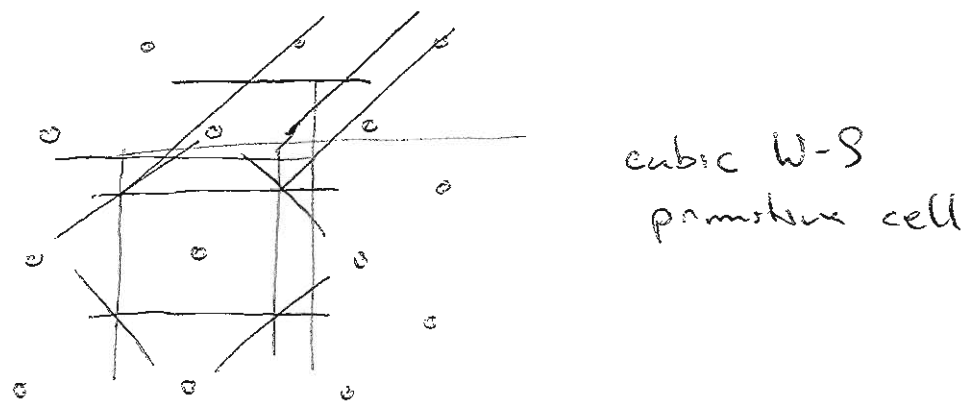




* Point is that the Wigner-Sertz Primitive Cell is advantageous from point of view of symmetry and is frequently used in theoretical works

~~caution~~ caveat: other primitive cells, such as parallelogram-type, are frequently used as well, depending on the need

simple cubic



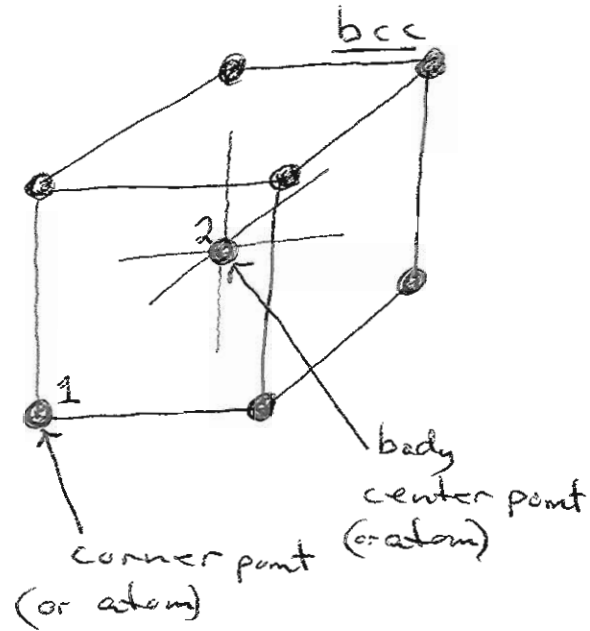
Crystal Structure: Lattice with a Basis

one use is to define certain Bravais lattices more simply

bcc

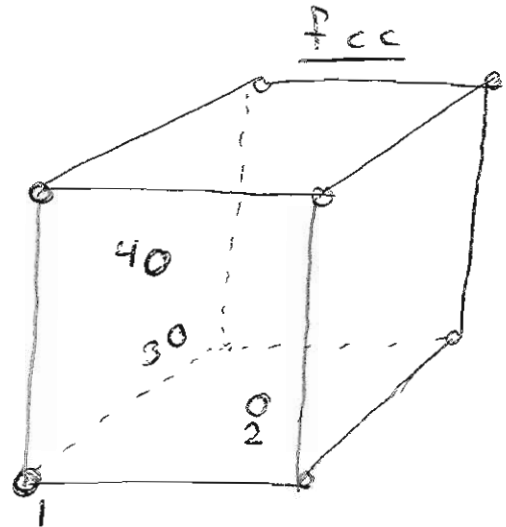
describe as just
SC + 2-~~point~~ basis

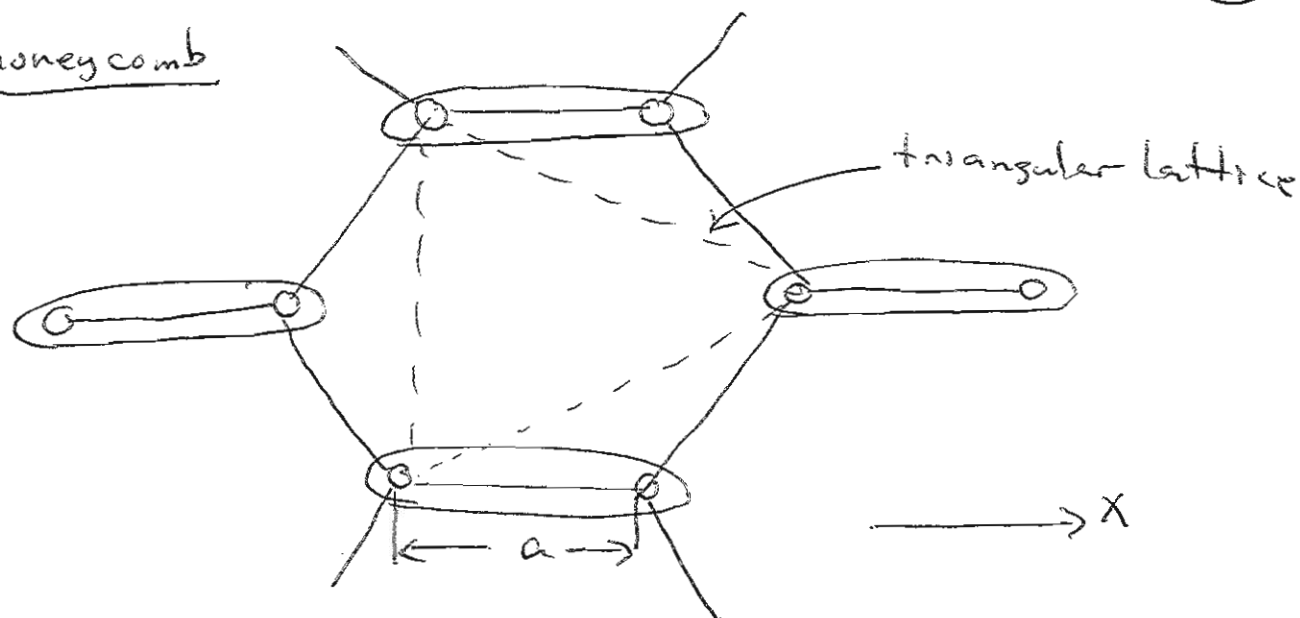
$$\begin{array}{cc} \frac{1}{(0,0,0)} & \frac{2}{\cancel{\frac{a}{2}(\hat{x}+\hat{y})} \quad \cancel{\frac{a}{2}(\hat{y}+\hat{z})}} \\ \text{or } \vec{0} & \frac{a}{2}(\hat{x}+\hat{y}+\hat{z}) \end{array}$$



similarly fcc

$$\begin{array}{cc} \frac{1}{(0,0,0)} & \frac{2}{\frac{a}{2}(\hat{x}+\hat{y})} \\ = \vec{0} & \\ \frac{3}{\frac{a}{2}(\hat{y}+\hat{z})} & \frac{4}{\frac{a}{2}(\hat{x}+\hat{z})} \end{array}$$



honeycomb

honeycomb can be viewed as (triangular or hexagonal lattice) + (2 point basis)

$$\frac{1}{\vec{0}}$$

$$\frac{2}{a \hat{x}}$$

Some important ~~examples~~ types of crystal structures which are not Bravais but which can be described as (Bravais) + (Basis of 2 or more points) or objects

- a. diamond structure
- b. zinc-blende (ZB)
- c. hexagonal close-packed (hcp)
- d. sodium chloride or rock-salt
- e. cesium chloride

diamond (D)

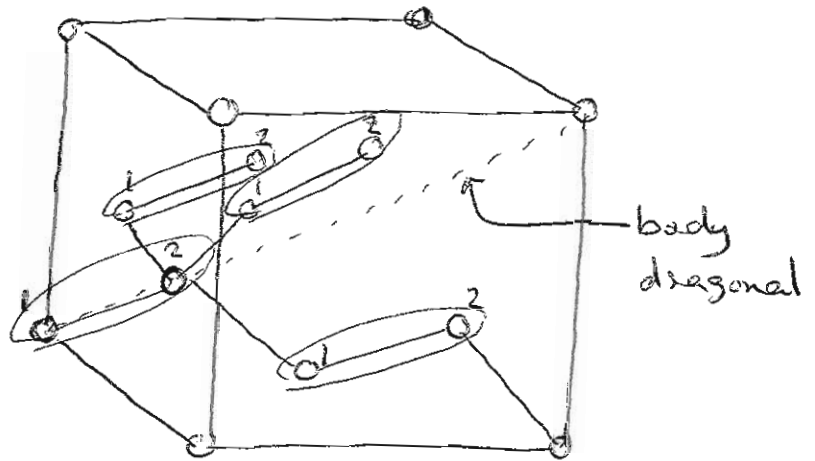
$$(D) = (\text{fcc Bravais}) + (2\text{-Point Basis})$$

$$\frac{1}{0}$$

$$\frac{2}{\frac{a}{4}(\hat{x} + \hat{y} + \hat{z})}$$

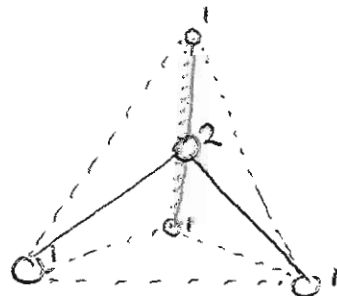
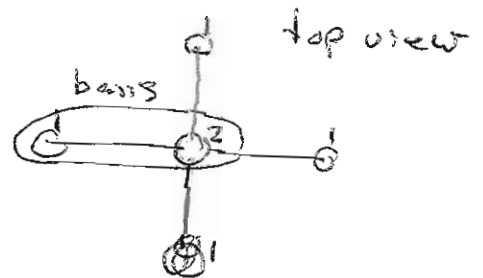
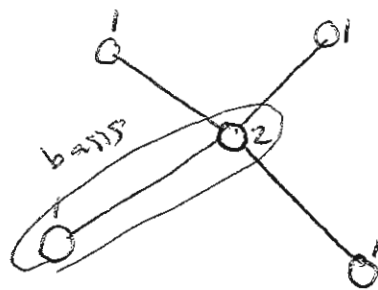
examples

- C (diamond)
- Si
- Ge
- α -Sn (grey)



Because of this basis, we get lattice sites which have 4 nearest neighbors in a tetrahedral arrangement

perspective view

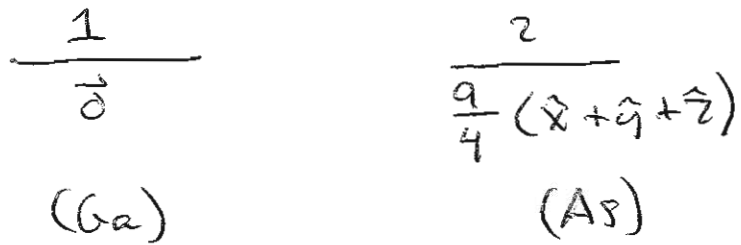


in the tetrahedron perspective, atoms of basis pt ① form the vertices of a tetrahedron, with atom of point ② at the center

Zinc-blend

(69)

same as diamond structure except that atoms of basis are of different element



\Rightarrow GaAs
ZnS (zinc-blende)
ZnSe
ZnTe
CdTe
AlAs
AlSb
GeP
GeSb
InP
InAs
InSb
+ more = lots

very important crystal structure

\Rightarrow many are direct gap materials with great technological applications

Sodium Chloride Structure

(70)

$$= (\text{fcc Bravais}) + (2\text{-atom basis})$$

$$\frac{1}{0}$$

(Na)

$$\frac{2}{\frac{a}{2}(\hat{x} + \hat{y} + \hat{z})}$$

(Cl)

\Rightarrow NaCl

LiF

LiCl

LiBr

KCl

MgO

ScN ! and several other transition metal nitrides

these materials are also of high practical applications,
many important uses to society

hexagonal close packing

(71)

$$\text{hcp} = (\text{hex Bravais}) + (\text{2-atom basis (pt.)})$$

$$\frac{1}{0}$$

$$\frac{2}{\frac{a_1}{3} + \frac{a_2}{3} + \frac{a_3}{2}}$$

