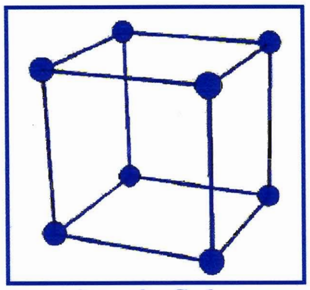
Solids encompass tremendous

- variety of properties
- number of elements and compounds

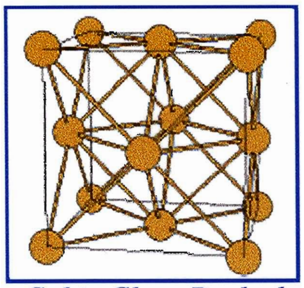
- Conductivities from ∞ (supercond.) to 10^{-16} $(\Omega\text{-cm})^{-1}$ [SiO_2]
- Optical properties (visible light)
  1) reflecting
  2) transparent
  3) absorbing
- Magnetic properties: para- dia- ferro- ferri- magnetic
- Mechanically hard (diamond) malleable (Pb)

....

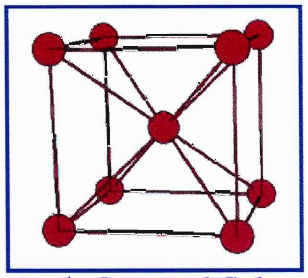
What is common?



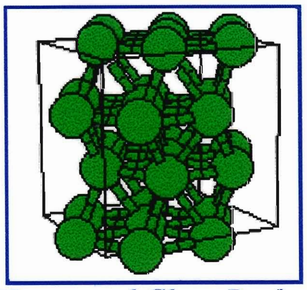
Simple Cubic
and related structures



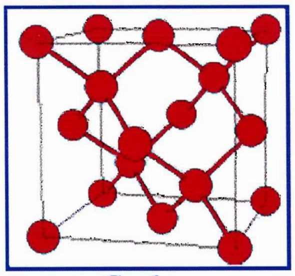
Cubic Close Packed
and related structures



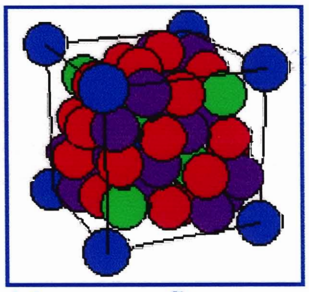
Body Centered Cubic
and related structures



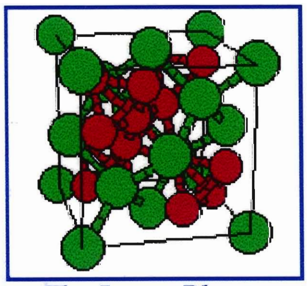
Hexagonal Close Packed
and related structures



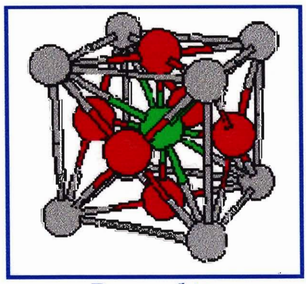
Carbon
and Related Structures



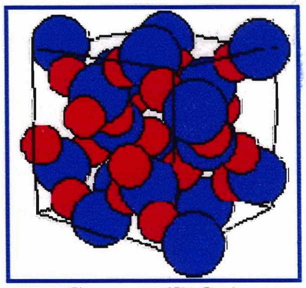
Manganese Structures



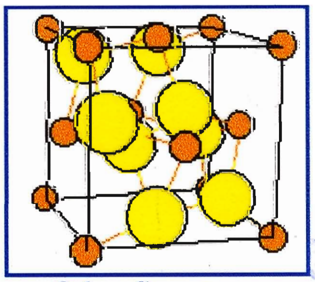
The Laves Phases



Perovskite
and Related Structures



Quartz (SiO_2)
and Related Structures



Other Structures

Structures indexed by:

1.2

Bravais lattice (BL)

(1) An infinite array of discrete points that appears exactly the same, from $\forall$ of the points is viewed

(2) A three-dimensional (3D) BL:

array of points with positions

$$\vec{R} = n_1 \cdot \vec{a}_1 + n_2 \cdot \vec{a}_2 + n_3 \cdot \vec{a}_3$$

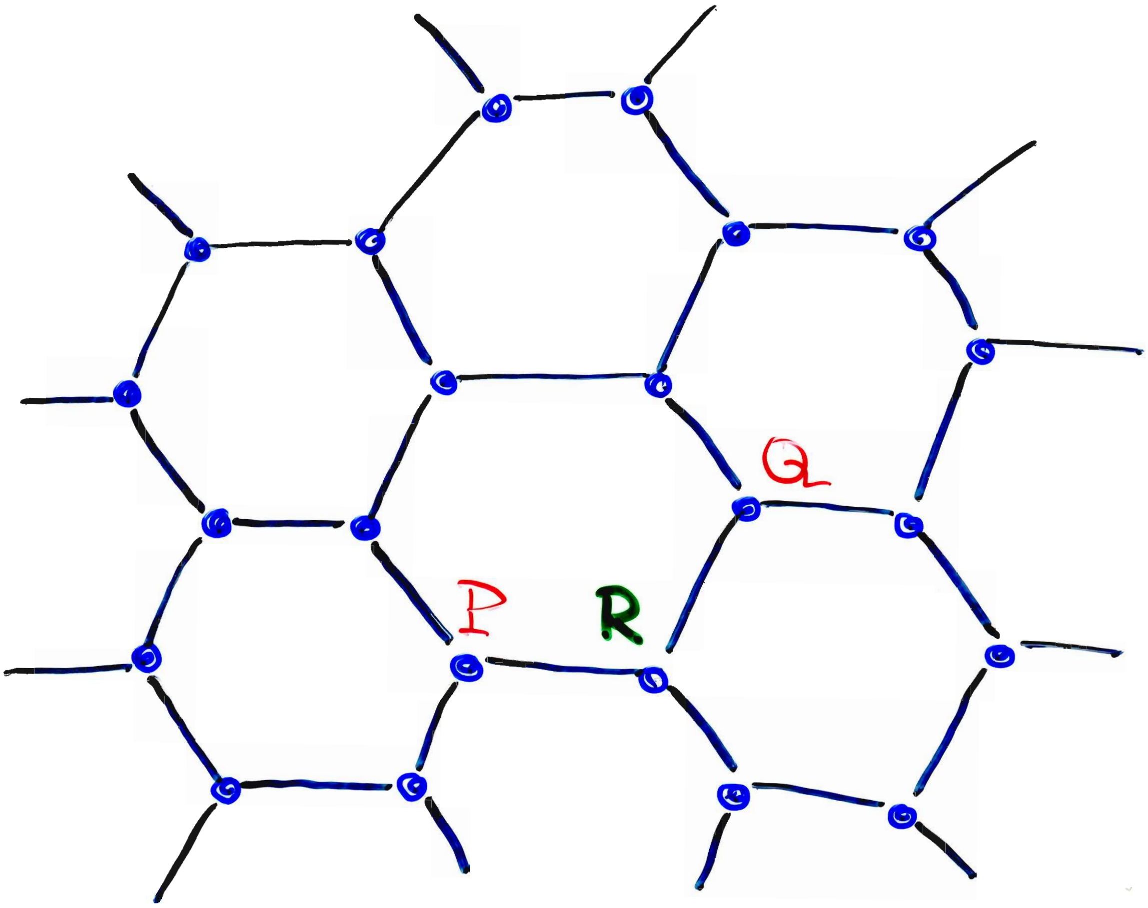
vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ are not in the same plane

called primitive vectors

$n_1\, n_2\, n_3$ are integers $0, \pm 1, \pm 2, \ldots$

$\vec{R}$ lattice translations

2D honeycomb. is BL?



Points P and Q equivalent

Points P and R are not:

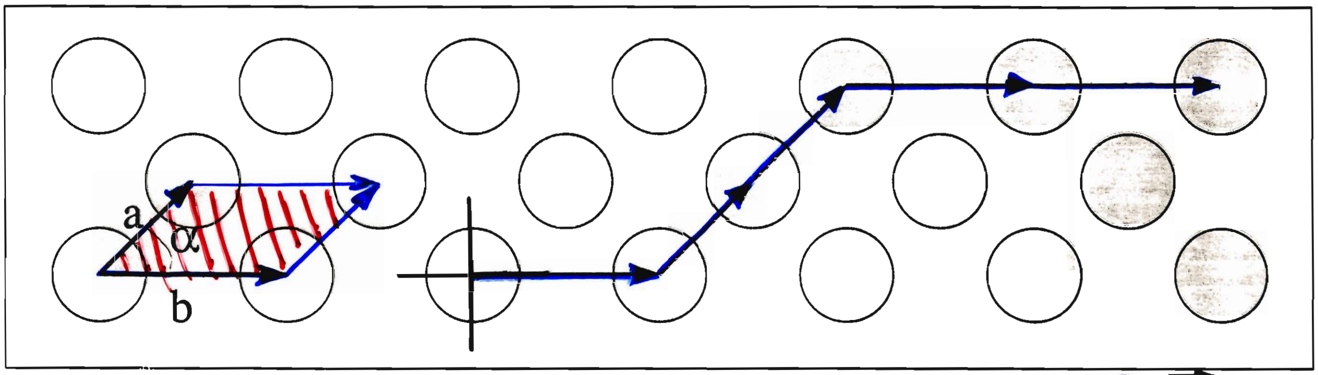
the views from P and R are *different*

$\boxed{\text{Not a BL!}}$

After rotation by $\underline{\pi}$

R becomes equivalent to P

(a portion of a) 2D BL of no particular symmetry (oblique net)

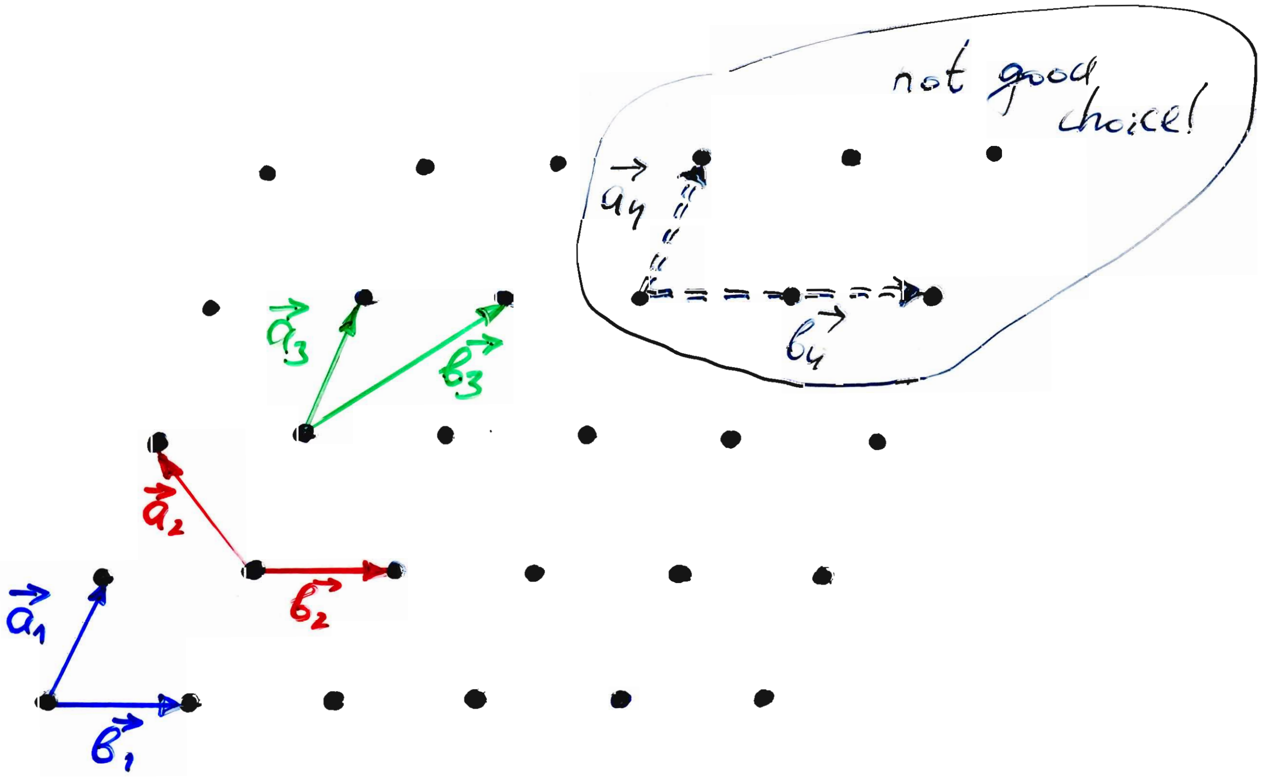


$\vec{R} = 2\vec{a} + 4\vec{b}$

Primitive cell like stacking building block

contains exactly <u>one</u> lattice point

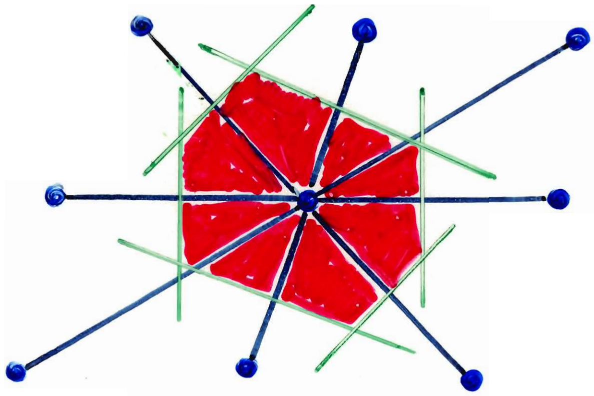
Area of PC $\quad S = |\vec{a} \times \vec{b}| = ab \sin\alpha$



Choice is not unique

1st BZ =

Wigner-Seitz Primitive Cell of the RL



k-space!

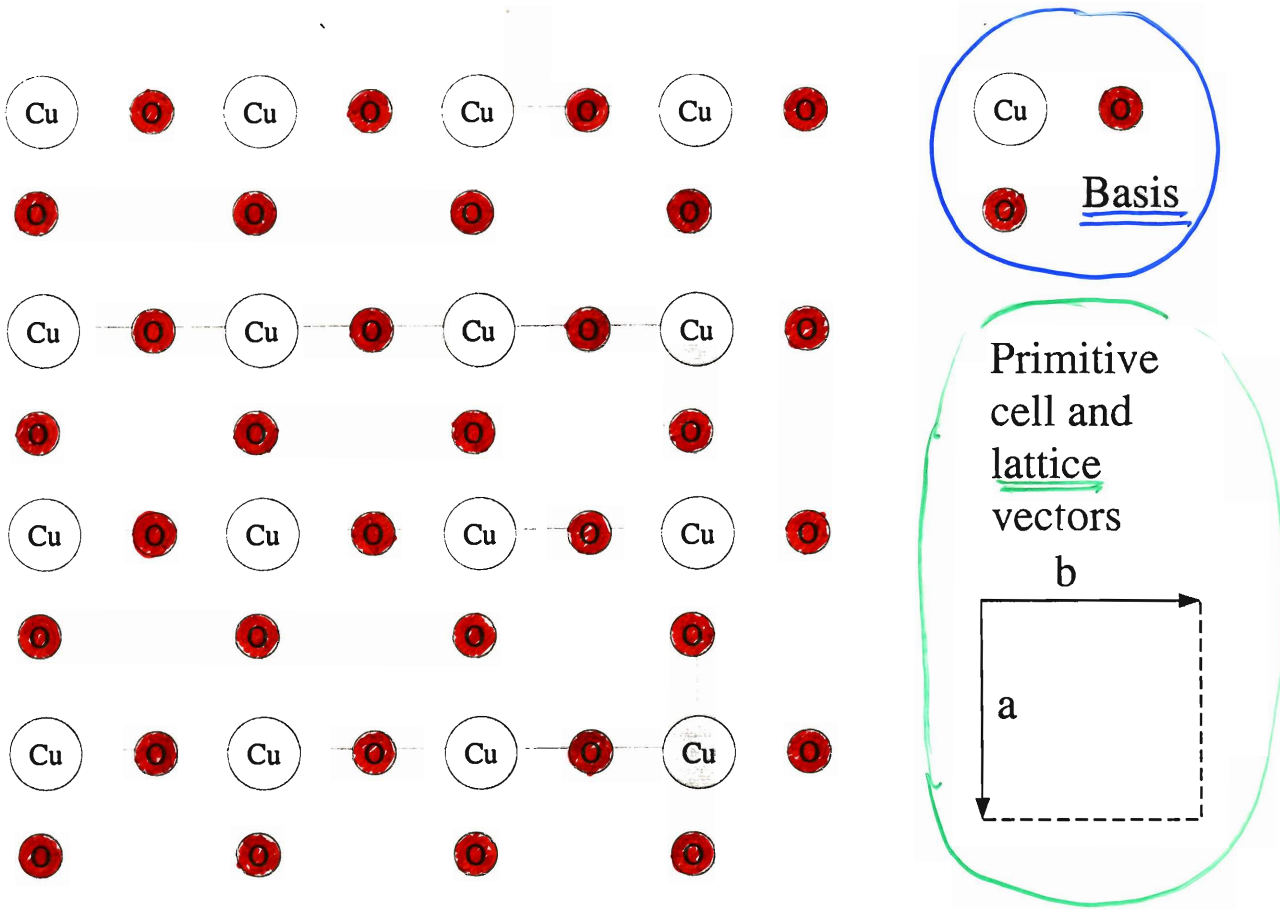
• lattice points

— lines connecting central point with nearest neighbors

| **perpendicular bisectrix**

WS unit cell = 1st BZ

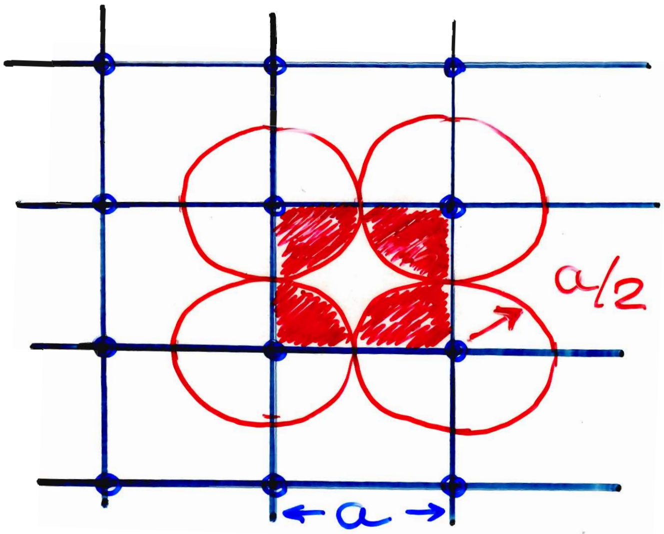
Possesses all the symmetries of lattice



Basis + Lattice = Crystal structure

Packing fraction P

2D square lattice



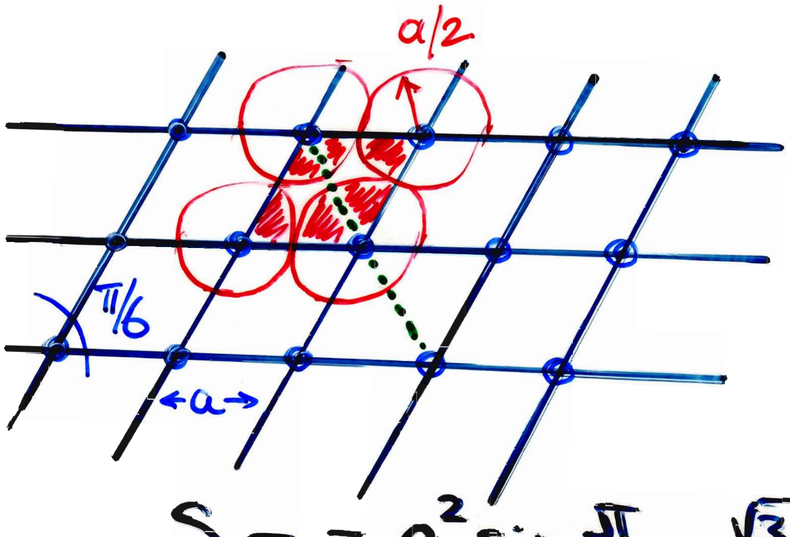
number of nearest neighbors
$\equiv$
coordination number

4

nearest-neighbor distance a

$$P_{\square}^{2D} = \frac{4 * \pi\left(\frac{a}{2}\right)^2 \cdot \frac{1}{4}}{a^2} = \frac{\pi}{4} \simeq 0.79$$

2D hexagonal lattice (jargon: triangular)



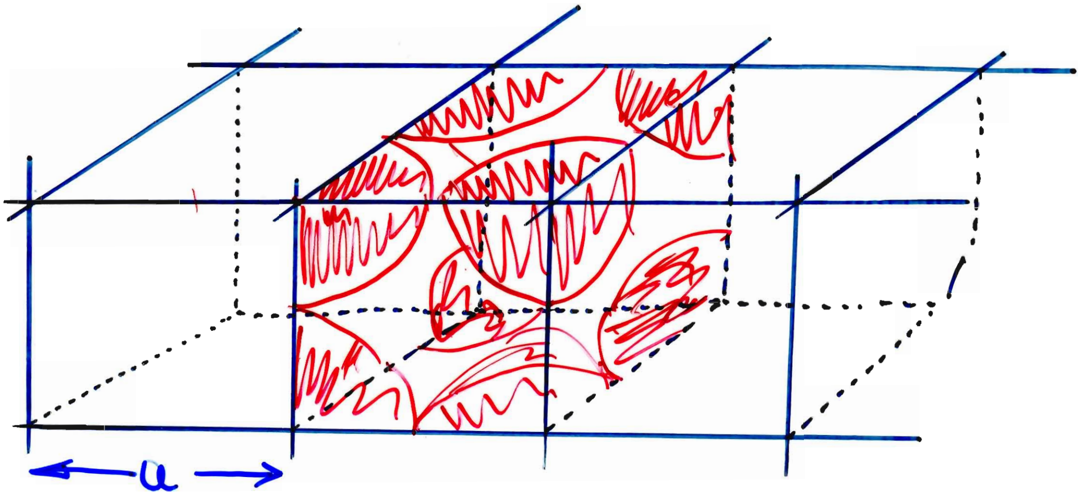
coordination number 6

nearest-neighbor distance a

$$S_{\varnothing} = a^2 \sin\frac{\pi}{6} = \frac{\sqrt{3}}{2} a^2$$

$$P_{\triangle}^{2D} = \frac{6 * \pi\left(\frac{a}{2}\right)^2 \cdot \frac{1}{6}}{\frac{\sqrt{3}}{2} a^2} = \frac{\sqrt{3} \cdot \pi}{6} \simeq 0.91$$

3D simple cubic (SC) lattice



coordination number 6
nearest-neighbor distance a

$$P^{3D}_{\square} = \frac{8 * \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 / 8}{a^3} = \frac{\pi}{6} \simeq 0.52$$

What are closed-packed lattices in 3D ?

Figure VI

BL lattice!

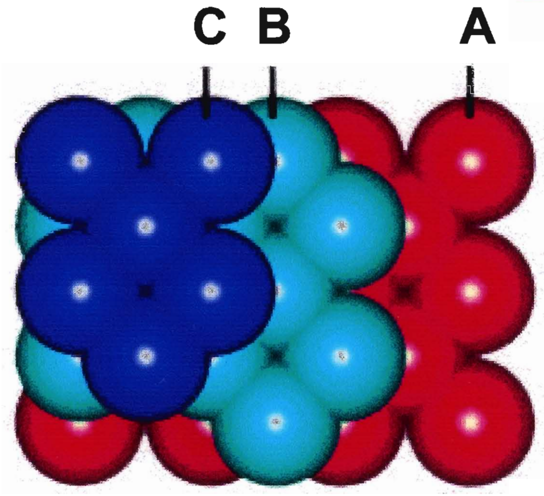
Face-Centered Cubic (FCC)

enormous variety of solids! Ar, Ag, Al, Cu

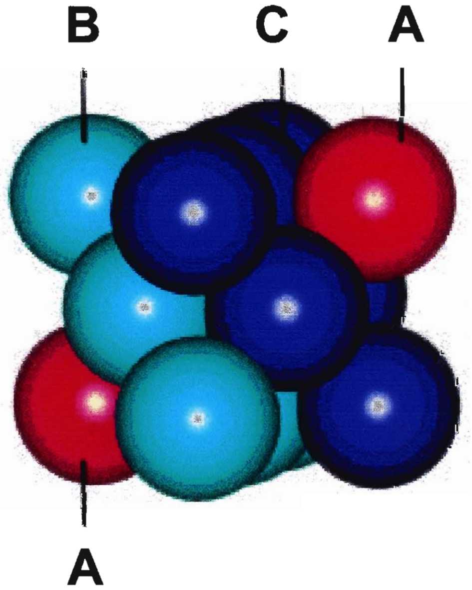
monatomic

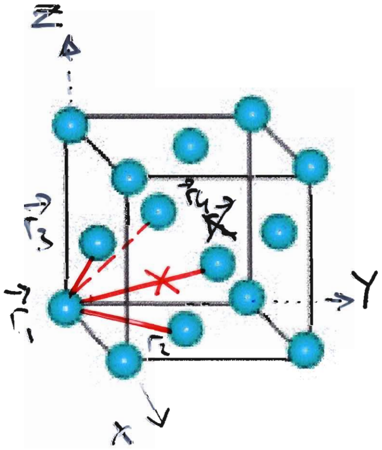
Close-packed structure

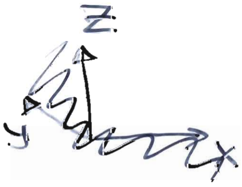
Coordination number 12



ABCABC...







can be also described as a simple cubic l. with a 4-point Basis

$\vec{r}_1 = 0 \quad \vec{r}_2 = \frac{a}{2}(\hat{x}+\hat{y}) \quad \vec{r}_3 = \frac{a}{2}(\hat{x}+\hat{z}) \quad \vec{r}_4 = \frac{a}{2}(\hat{y}+\hat{z})$

FCC

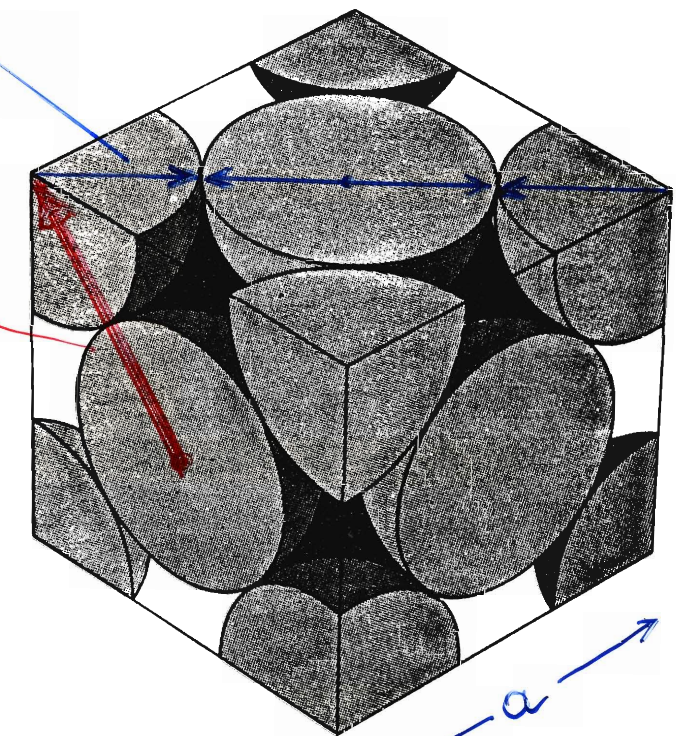
$$V_{filled} = \left[8 * \frac{1}{8} + 6 * \frac{1}{2}\right] \cdot \frac{4\pi}{3} r^3 = 4 \cdot \frac{4\pi}{3}\left(\frac{\sqrt{2}a}{4}\right)^3$$

$$\text{Packing fraction} = \frac{V_{filled}}{a^3} = \frac{\sqrt{2}\,\pi}{6} \simeq 0.74$$

$r = \frac{\sqrt{2}a}{4}$

nearest-neighbor distance

$\frac{\sqrt{2}a}{2}$



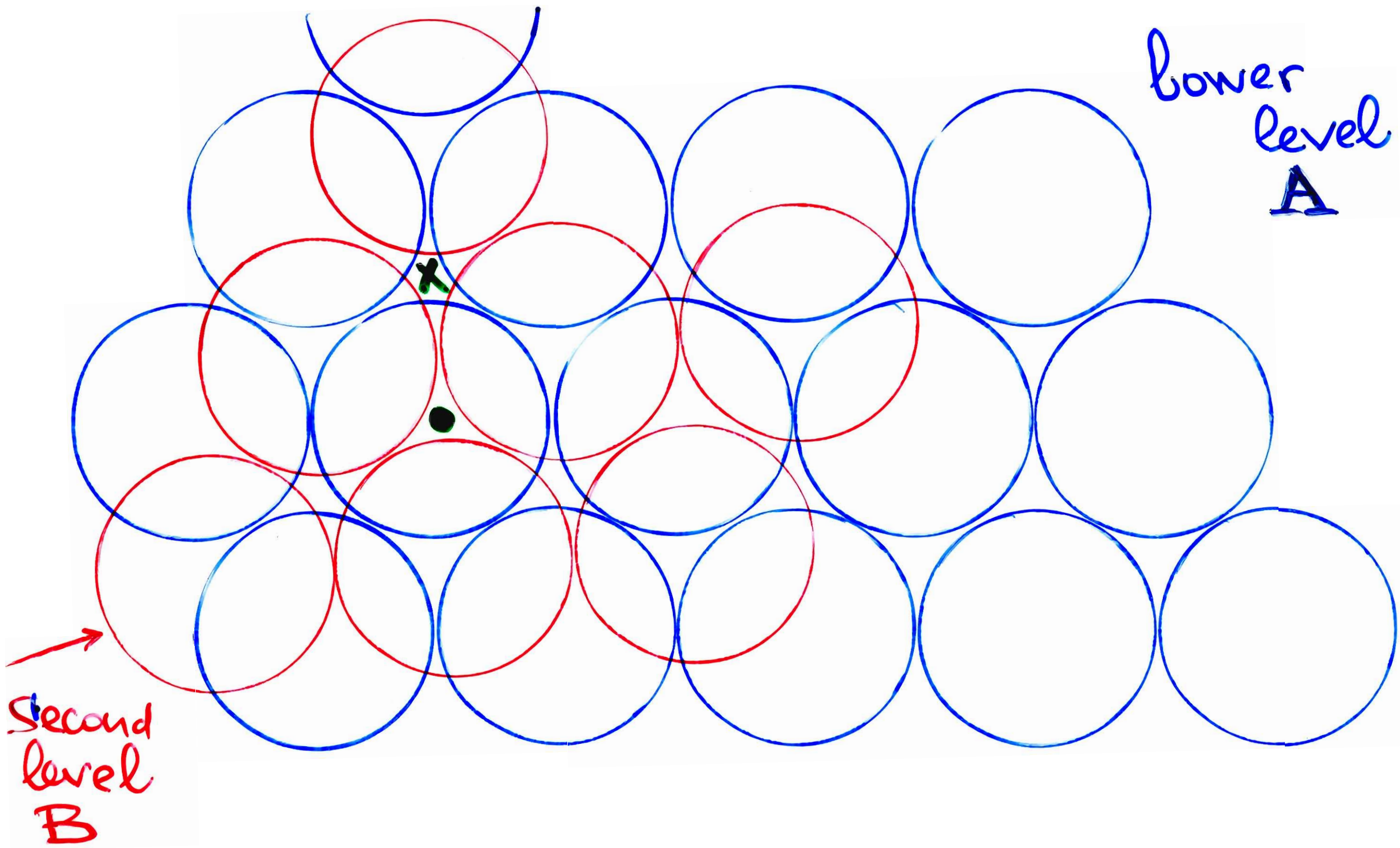
a

FCC <u>conventional</u> cell $V = a^3$

contains <u>4</u> atoms

primitive cell $V_p = \frac{1}{4}a^3$

Stacking cannon balls...



where to put 3rd level?

two choices: X or •

ABC ABA

∞ number of ways to continue....

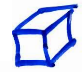
e.g. ABABC...

Only ABCABCABC...

gives a Bravais lattice:

Face-centered cubic FCC

ABAB... → hexagonal close-packed

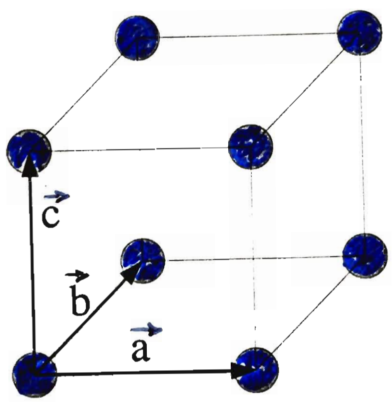


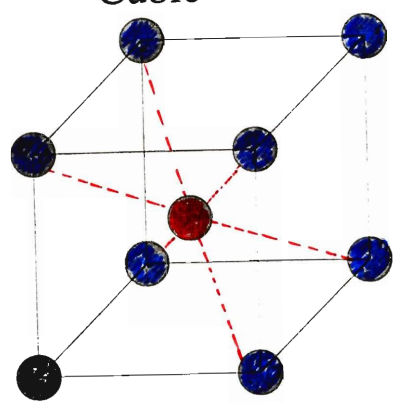
Volume, conventional cell a^3

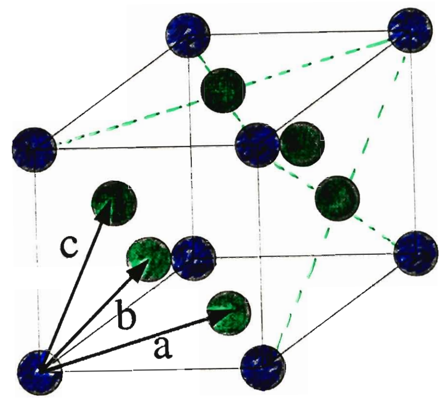
CUBIC

1.2 Three-Dimensional Lattices

SC	BCC	FCC
simple Cubic	Body Centered Cubic	Face Centered Cubic







SC	BCC	FCC
$\vec{a} = \hat{x} \cdot a$	$\vec{a} = (\hat{x}+\hat{y}-\hat{z})/2 \cdot a$	$\vec{a} = (\hat{x}+\hat{y})/2 \cdot a$
$\vec{b} = \hat{y} \cdot a$	$\vec{b} = (-\hat{x}+\hat{y}+\hat{z})/2 \cdot a$	$\vec{b} = (\hat{x}+\hat{z})/2 \cdot a$
$\vec{c} = \hat{z} \cdot a$	$\vec{c} = (\hat{x}-\hat{y}+\hat{z})/2 \cdot a$	$\vec{c} = (\hat{y}+\hat{z})/2 \cdot a$

$$\boxed{\text{Volume, primitive cell } V = |\vec{a} \times \vec{b} \cdot \vec{c}|}$$

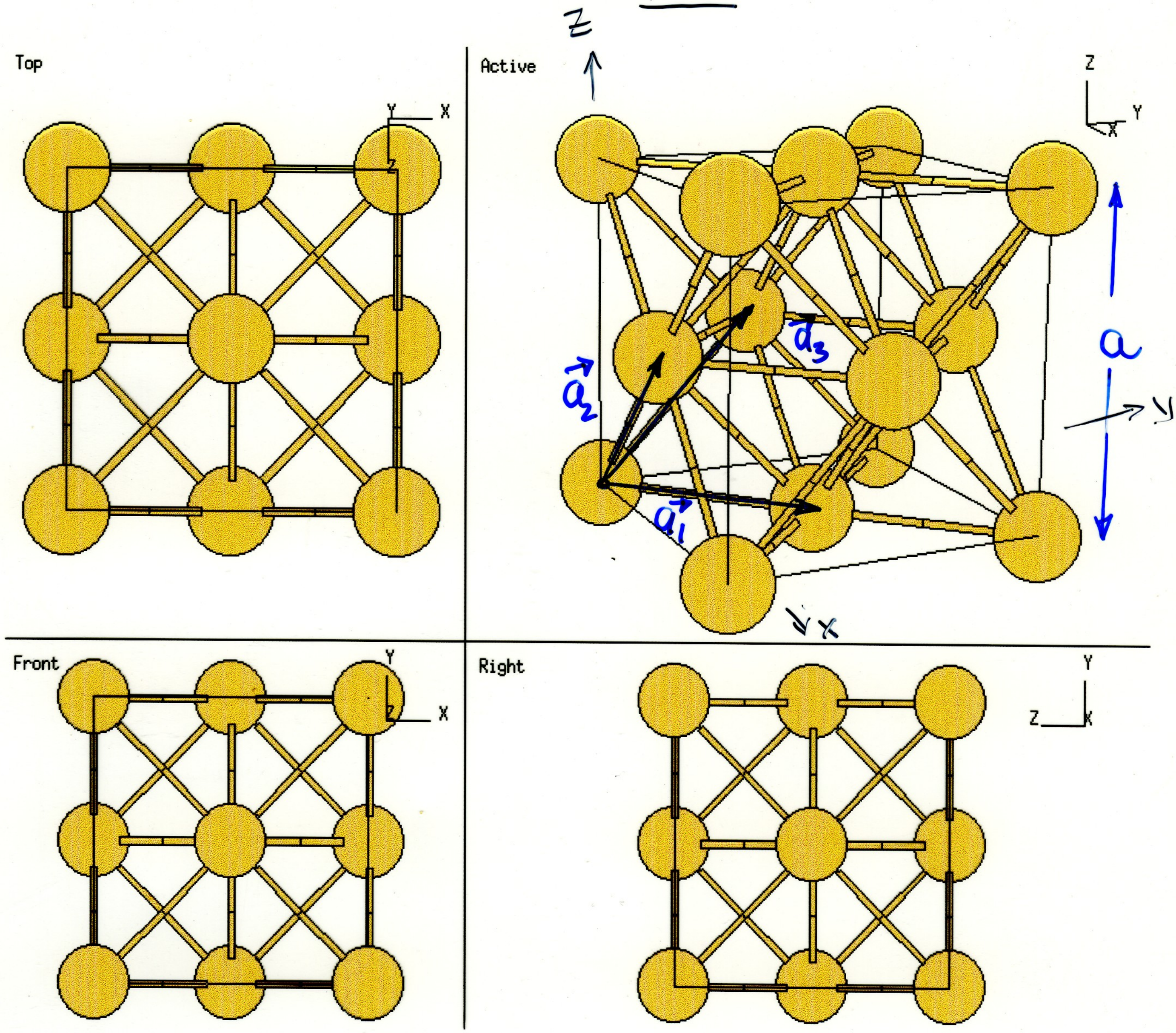
$V_{SC} = a^3$ $\qquad$ $V_{BCC} = \frac{1}{2} a^3$ $\qquad$ $V_{FCC} = \frac{1}{4} a^3$

$$\boxed{\text{Coordination number} \equiv \text{number of nearest neighbors}}$$

6 $\qquad$ 8 $\qquad$ 12

	Nearest neighbor distance	
a	$\frac{\sqrt{3}a}{2} \simeq 0.87a$	$\frac{\sqrt{2}a}{2} \simeq 0.71a$
$P_{SC} = \frac{\pi}{6} \simeq 0.52$	$P_{BCC} = \frac{\sqrt{3}\pi}{8} \simeq 0.68$	$P_{FCC} = \frac{\sqrt{2}\pi}{6} \simeq 0.74$

FCC



Primitive vectors

$$\vec{a}_1 = \frac{1}{2}a(\hat{x}+\hat{y})$$

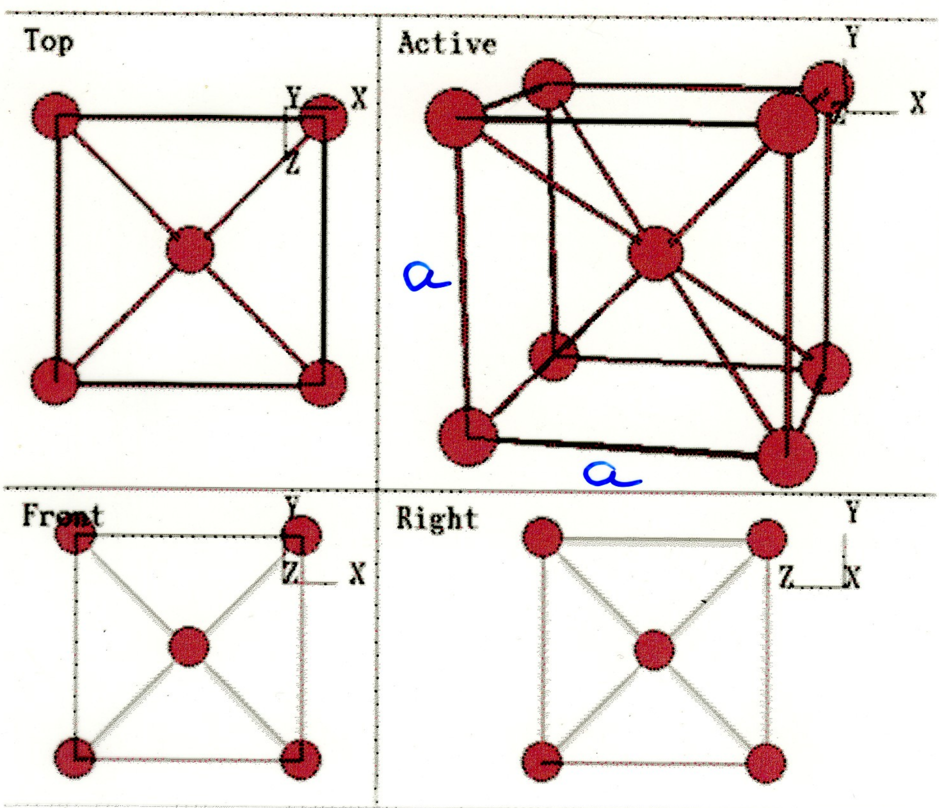
$$\vec{a}_2 = \frac{1}{2}a(\hat{x}+\hat{z})$$

$$\vec{a}_3 = \frac{1}{2}a(\hat{y}+\hat{z})$$

$$V_p = \frac{1}{4}a^3$$

(Monatomic) Body-Centered Cubic (BCC)

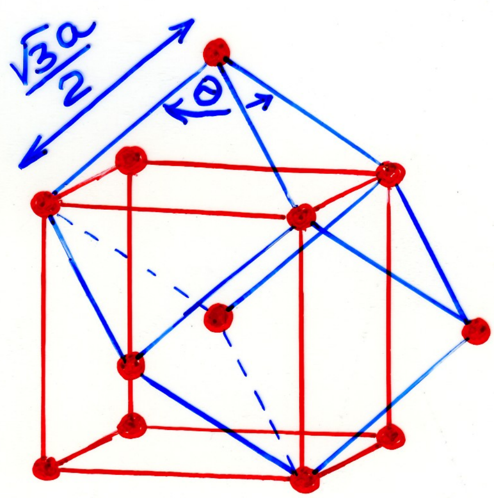
W, V, Tl, Ba, Cr, Cs, K, Li, ...

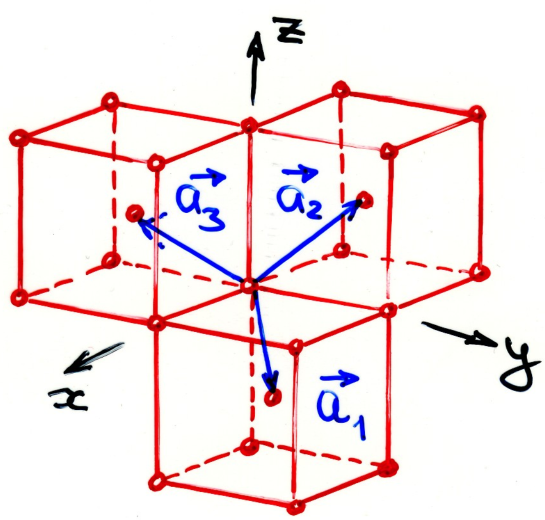


coordination number 8

nearest-neighbor distance

$$\frac{\sqrt{3}a}{2}$$





Primitive cell

RomBohedron

$\Theta = 109°28'$

Primitive vectors

$$\vec{a}_1 = \tfrac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$$

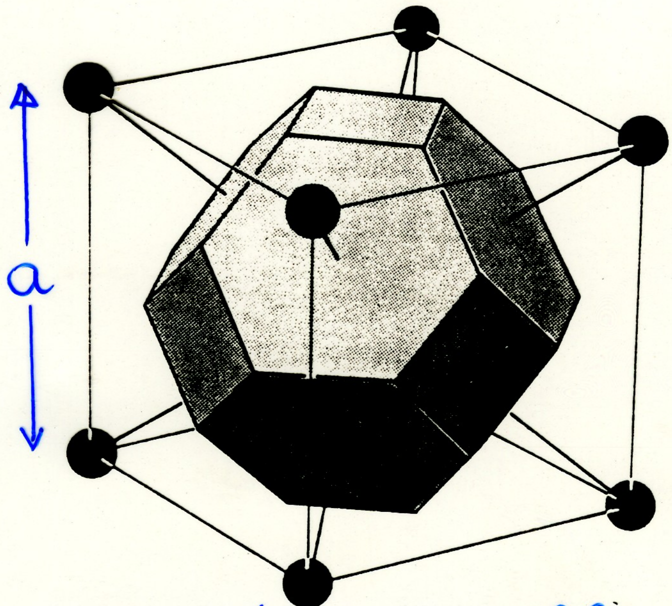
$$\vec{a}_2 = \tfrac{1}{2}a(-\hat{x}+\hat{y}+\hat{z})$$

$$\vec{a}_3 = \tfrac{1}{2}a(\hat{x}-\hat{y}+\hat{z})$$

$$V = \tfrac{1}{2}a^3$$

Wigner-Seitz Cell For

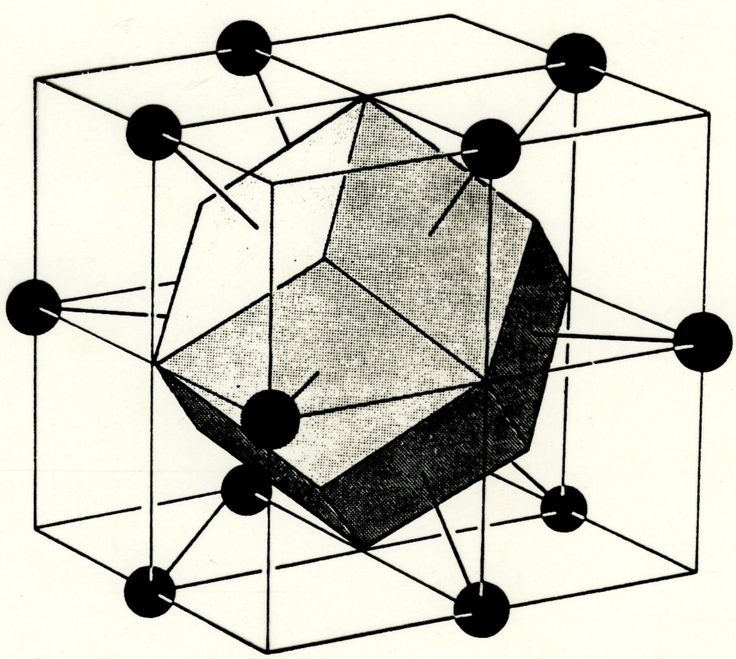
BCC



"truncated octahedron"

conventional cell

FCC

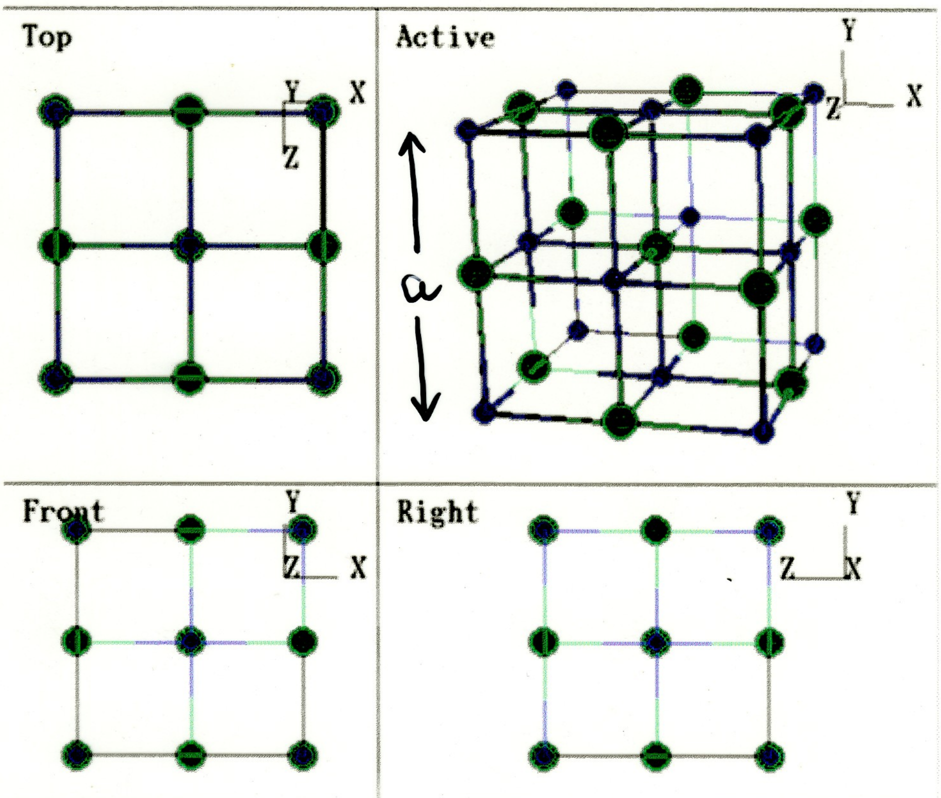


"rhombic dodecahedron"

not a conventional cell

Sodium Chloride Structure

$NaCl$, $AgCl$, CaO, KBr, ...

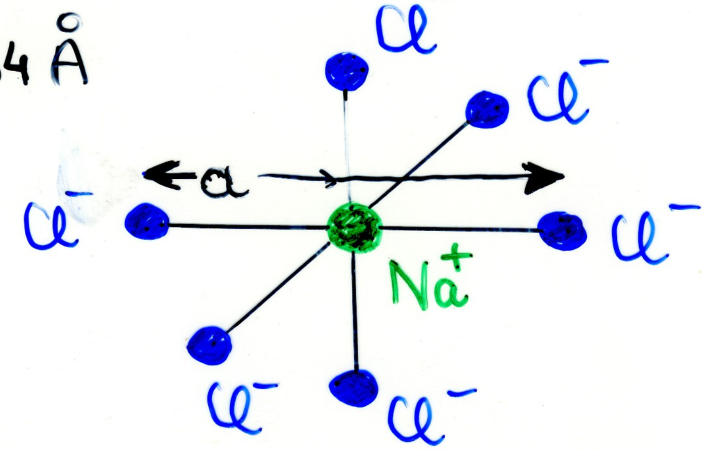


lattice constants: numbers specifying the size of a unit cell

A lattice with a basis: FCC with a two-point basis

different kinds of ions (e.g. Na^+ and Cl^-) are placed at alternate points of a simple cubic lattice

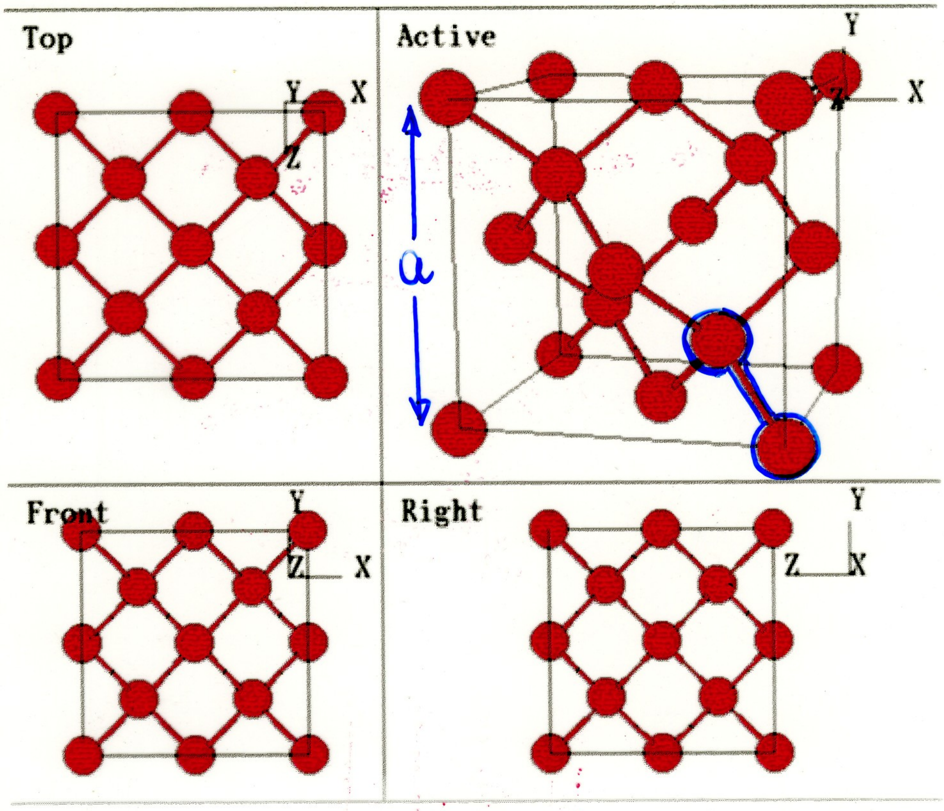
$a = 5.64$ Å

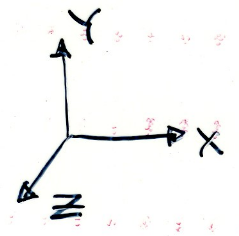


coordination number 6

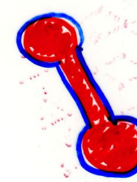
Diamond Crystal Structure

C (diamond), Si, Ge, Sn



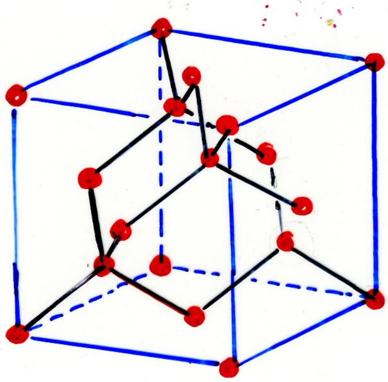


FCC with a two-point basis



$\frac{a}{4}(-1,1,-1)$

000



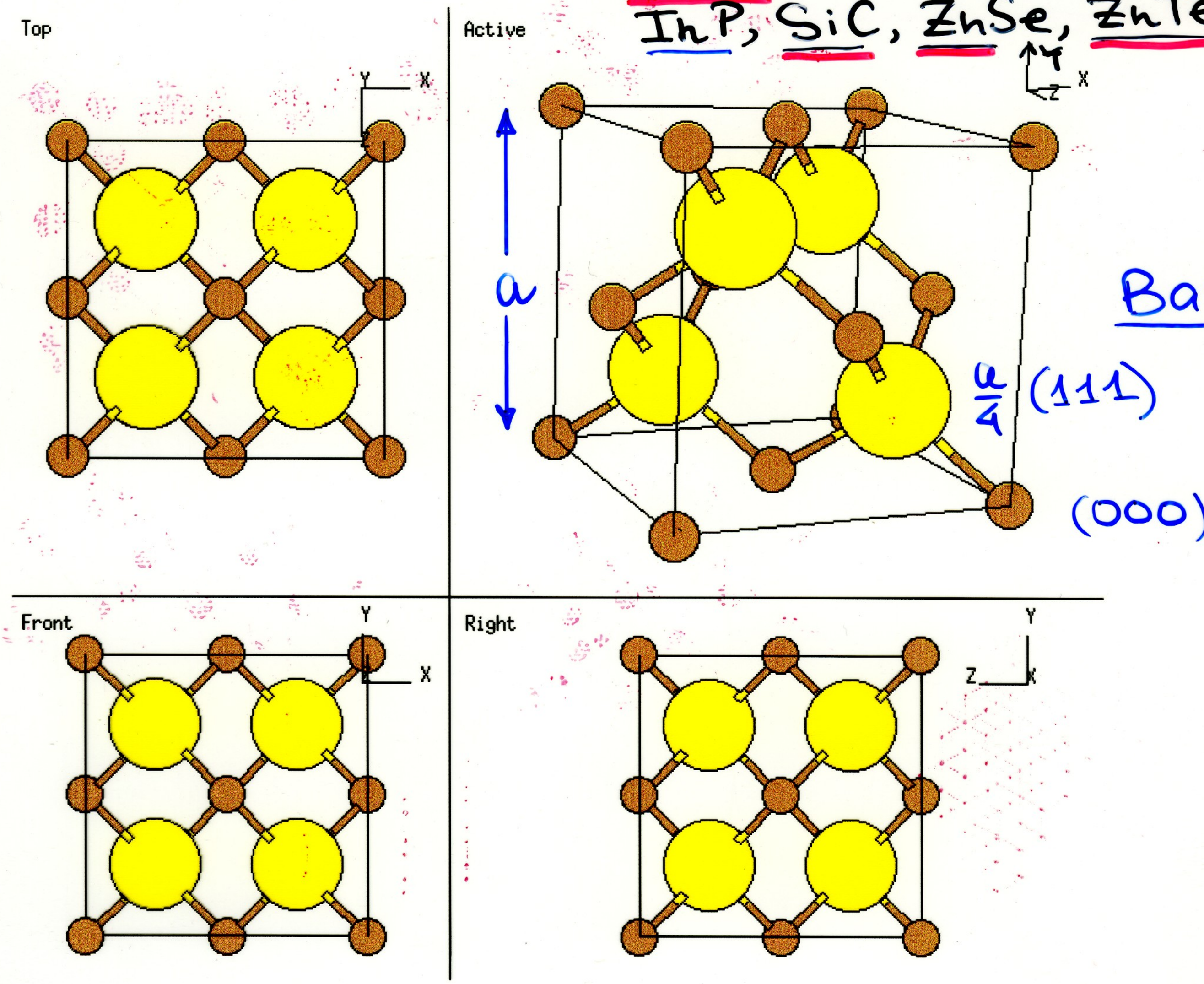
directional covalent
tetrahedral bonding

coordination number
4

18.8 / 2.9

Zincblende Structure

ZnSe, AlAs, GaAs, HgTe, InP, SiC, ZnSe, ZnTe...



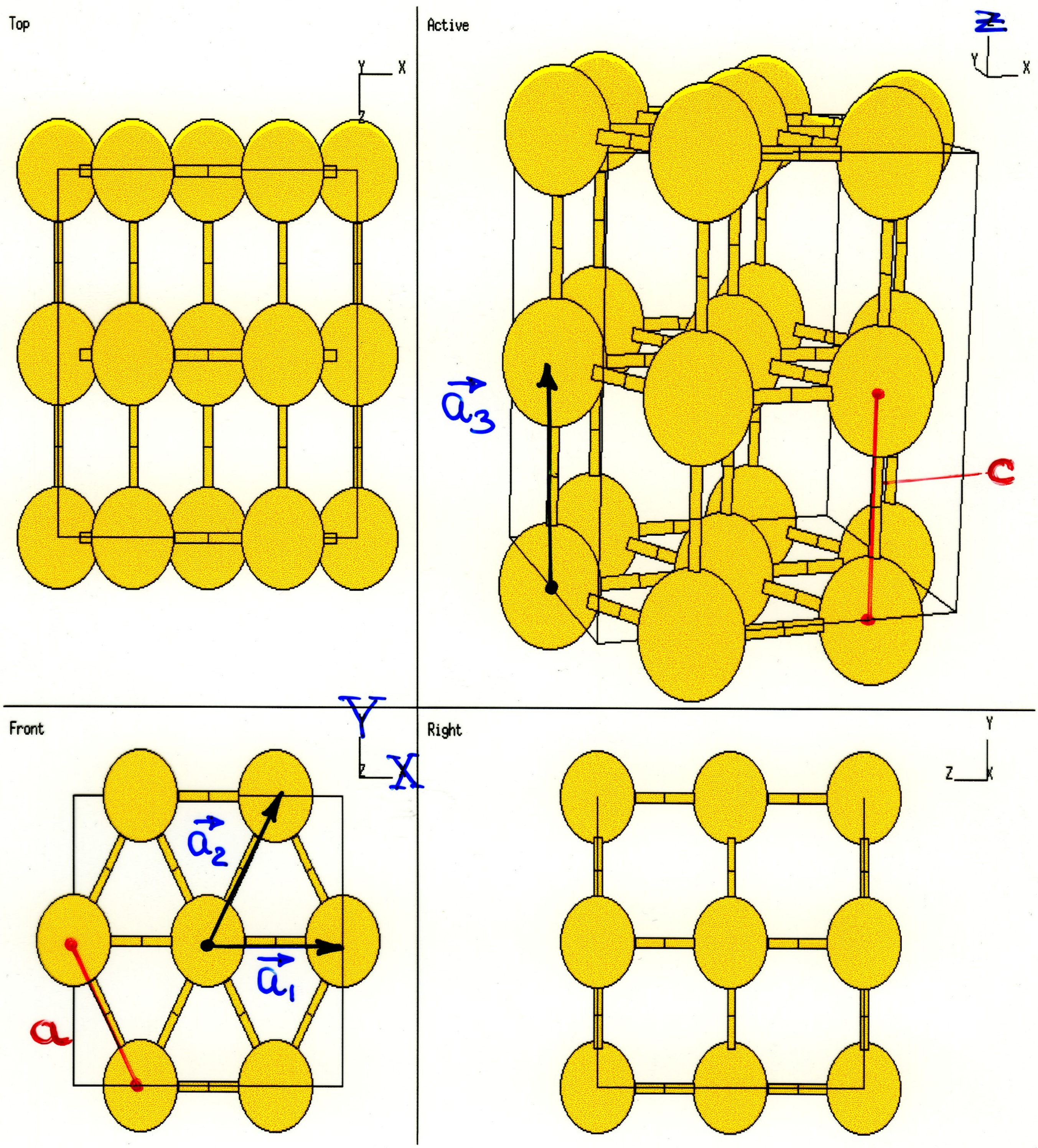
Basis

Two interpenetrating FCC lattices displaced by $\frac{1}{4}$ of the body diagonal

All $\overline{\text{III}}$-$\overline{\text{V}}$ compound S.C.

Some $\overline{\text{II}}$-$\overline{\text{VI}}$ compound S.C

Simple hexagonal BL (no elements in the ground state)

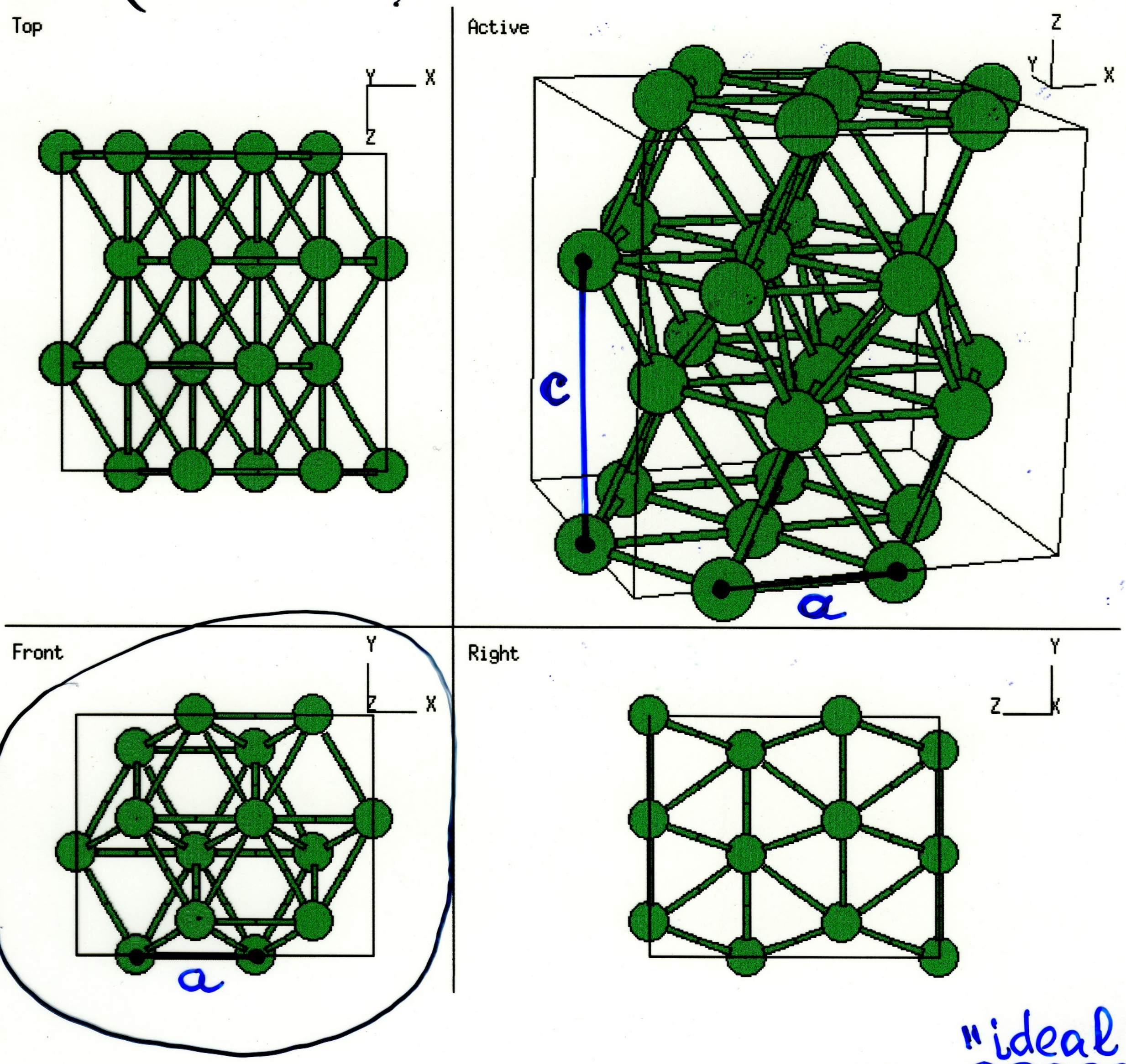


$$\vec{a}_1 = a\hat{x} \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y} \qquad \vec{a}_3 = c\hat{z}$$

$$V_p = |(\vec{a}_1 \times \vec{a}_2)\cdot\vec{a}_3| = \frac{\sqrt{3}}{2}a^2c$$

Hexagonal Close-Packed (HCP) (not BL!)

Be, Cd, ..., Mg, ...
He (2K), ...



"ideal HCP"

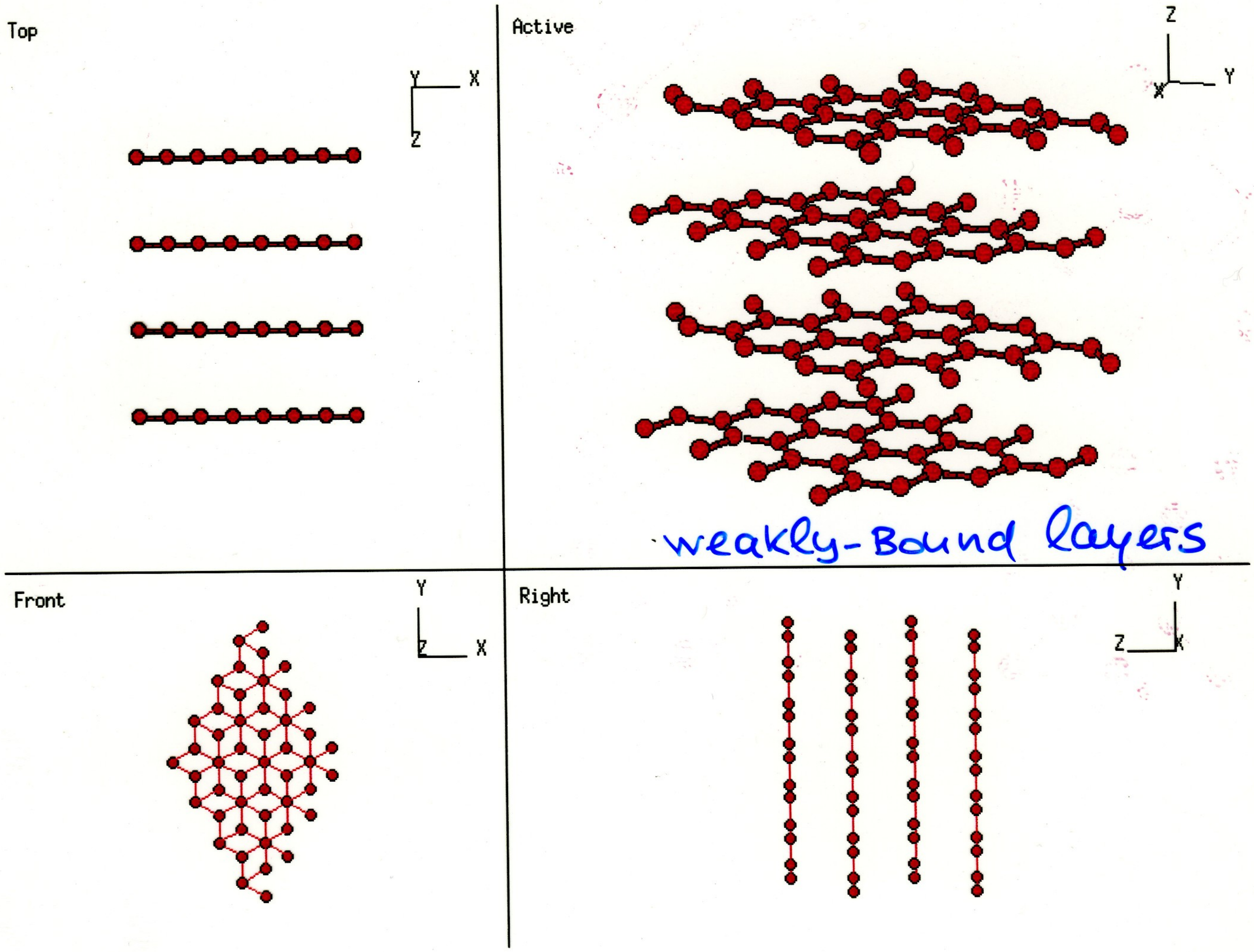
Close-packed when $c = \sqrt{\frac{8}{3}}\, a \simeq 1.63\, a$

Two interpenetrating simple hexagonal BLs

Two types of planes merge to form the 2D honeycomb

Graphite Crystal Structure

C (graphite)



weakly-Bound layers

2D Graphene

Nobel Prize 2010

three-connected

"sp^2 carbons" : one double and two single bonds

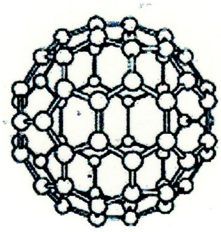
hexagons

planar structure cannot be closed having only hexagons

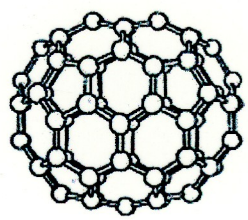
Return [first] [prev] [Cees Dekker, Delft Univ of Tech 04] [NEXT] [last]

Fullerenes

C60

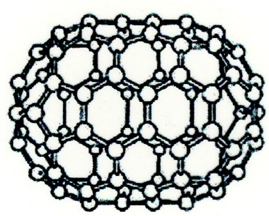


C70

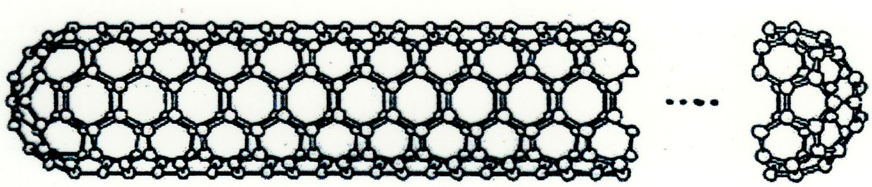


other stable
hollow
structures

C80 isomer

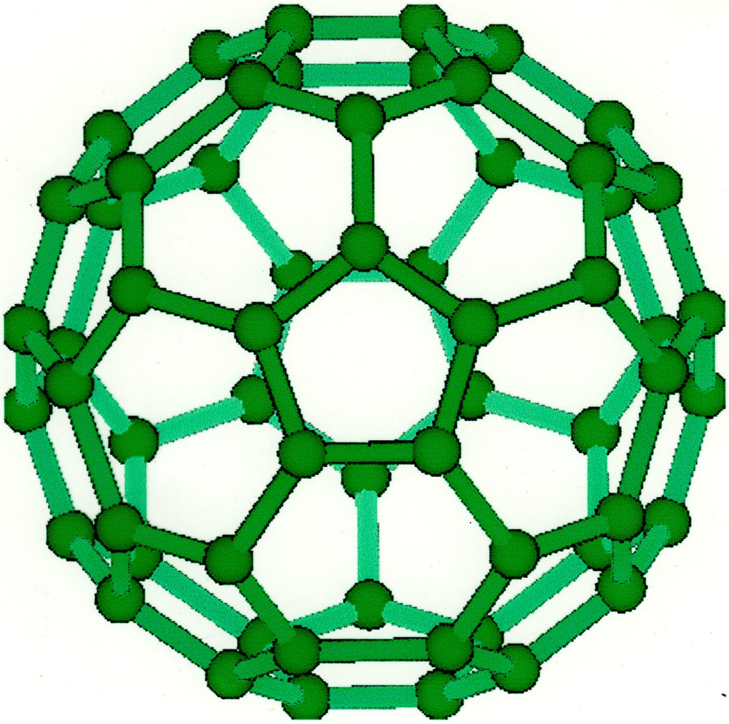


nanotube



quantum nano-wires
diameter ~ few nm
lengths 1-10 μm
can be metallic!

- 1D physics
- metallic contacts between wires etc.

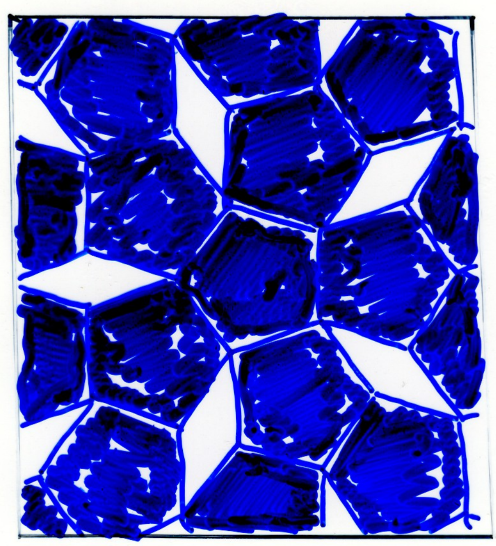


C_{60} "Fulleren"

interesting symmetries possible on a sphere!

hexagons + pentagons
∀ number 12 for closure

Nobel Prize in Chemistry 1996

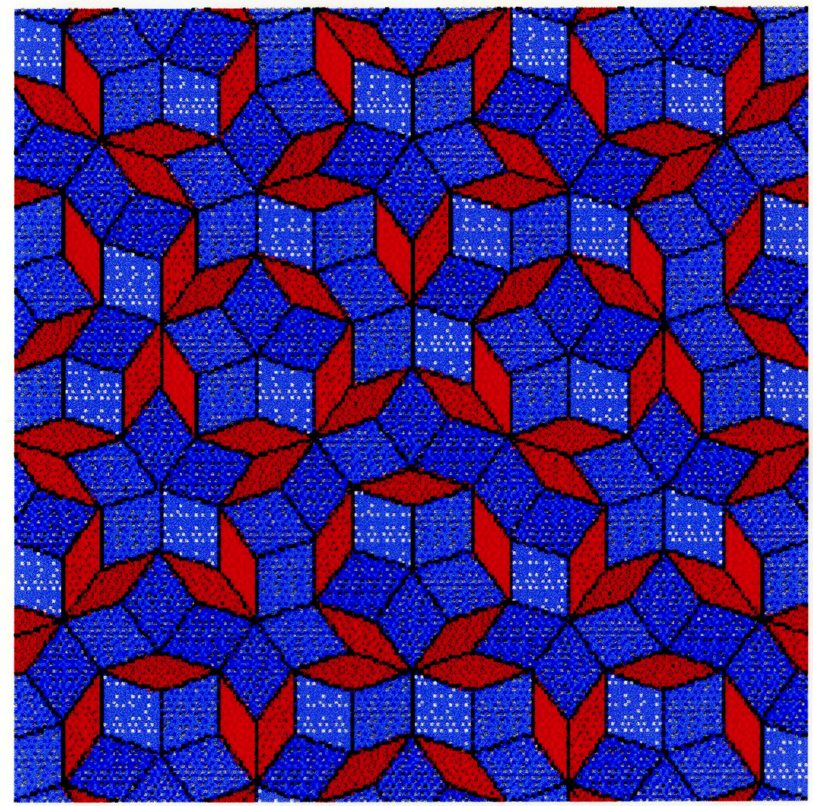


a lattice with a fivefold axis is not possible on a plane:
rotations $\frac{2\pi}{5}$ and translations are not compatible

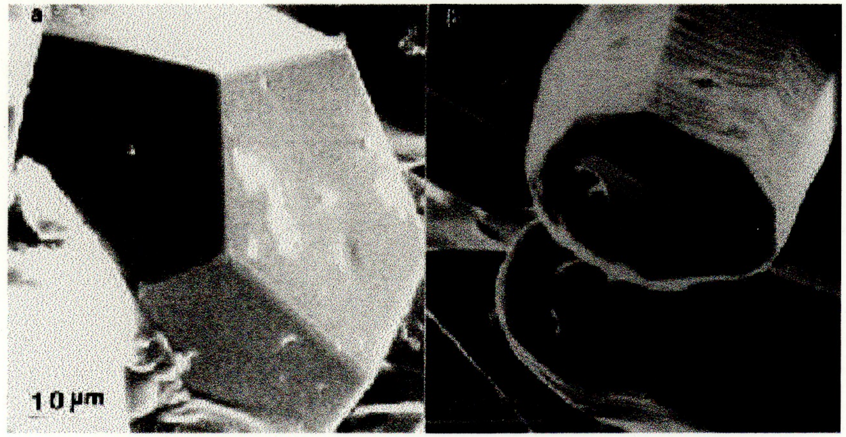
2.16

Quasicrystals

Quasicrystal structures don't have a simple "unit cell" that can be repeated periodically in all directions to fill space, although they do have local patterns that repeat almost periodically. They also have local rotational symmetries – such as those of a pentagon – that cannot exist in ordinary crystals. The best known examples *resemble* so-called **Penrose tilings**, which use repeated copies of two different rhombi to cover an infinite plane in intricate, interlocking patterns.



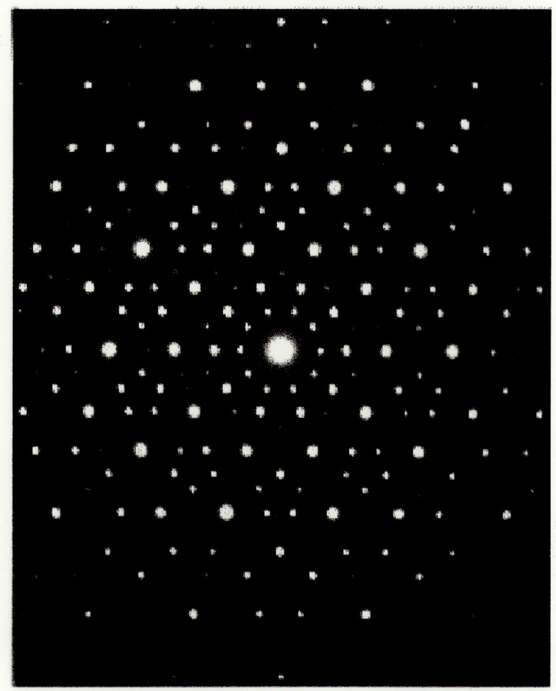
A Penrose tiling



an AlCuFe alloy an AlNiCo alloy

single grains of quasicrystals

In 1991, the International Union of Crystallography decided to redefine the term "crystal" to mean any solid having an *essentially discrete diffraction diagram*



Typical diffraction diagram of a quasicrystal, exhibiting 5-fold or 10-fold rotational symmetry.

Dan Shechtman (1982)

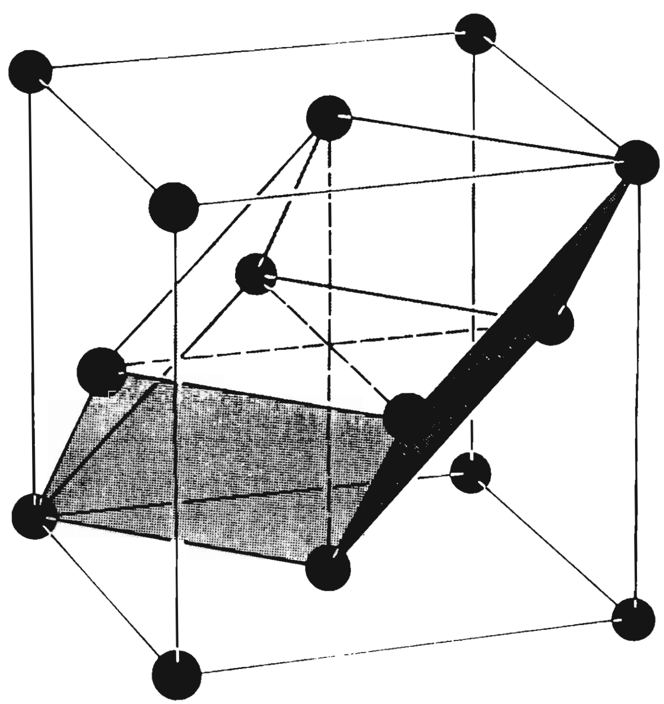


Figure 4.12
Primitive and conventional unit cells for the face-centered cubic Bravais lattice. The conventional cell is the large cube. The primitive cell is the figure with six parallelogram faces. It has one quarter the volume of the cube, and rather less symmetry.