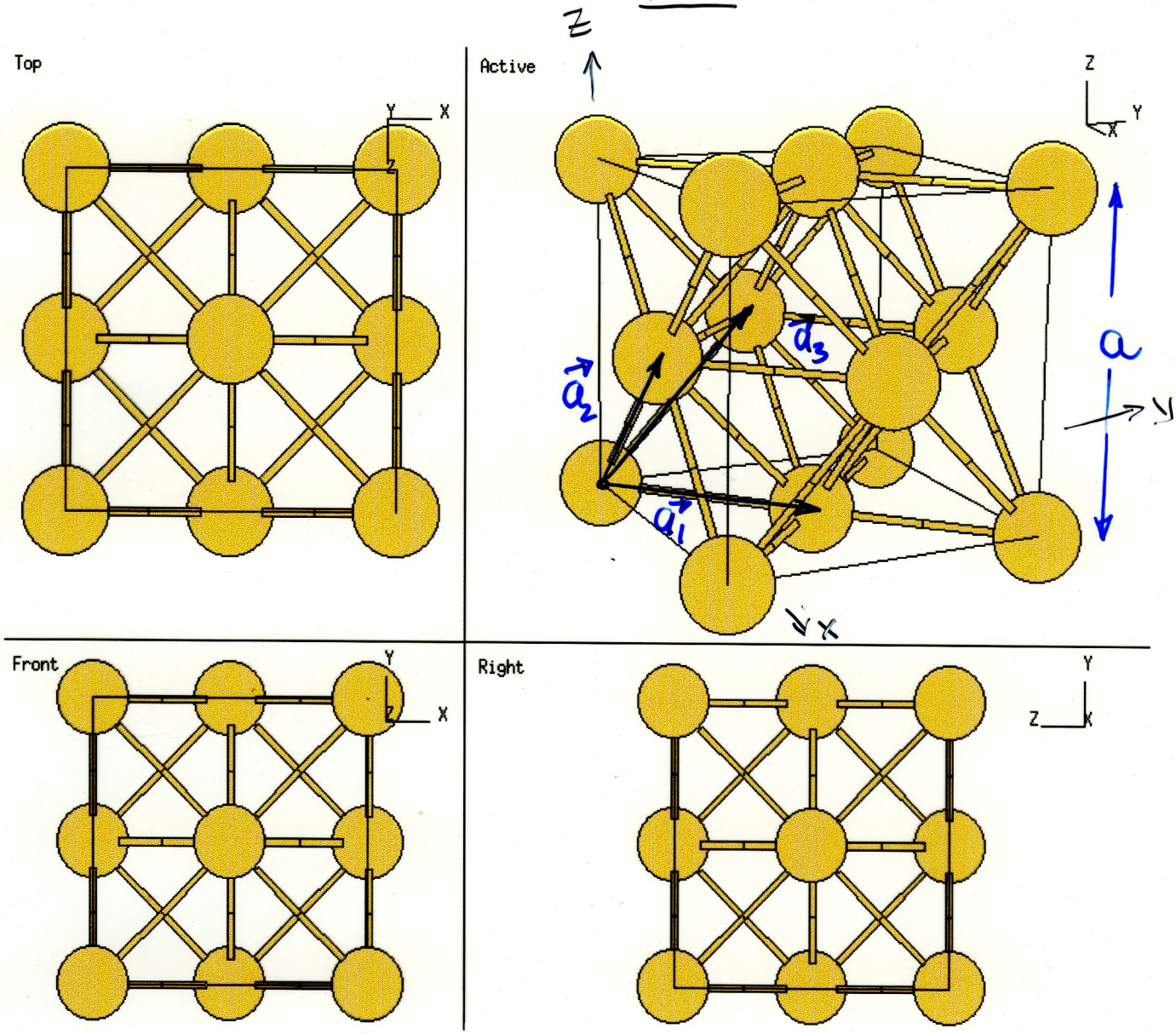
FCC



Primitive vectors

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

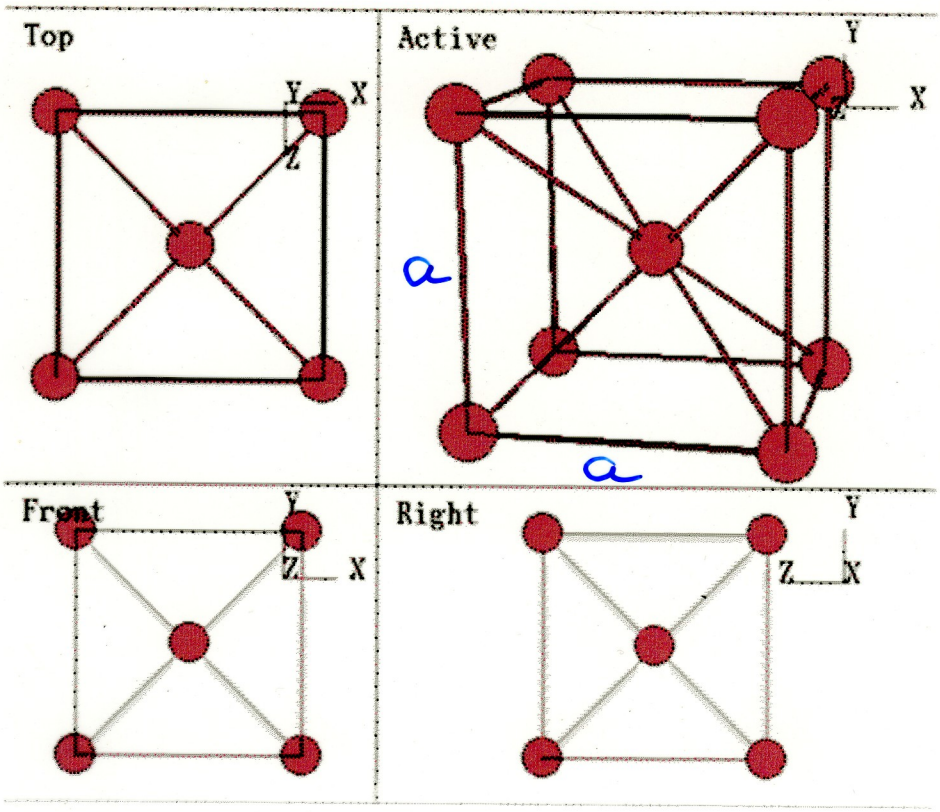
$$\vec{a}_2 = \frac{1}{2}a(\hat{x}+\hat{z})$$

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

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

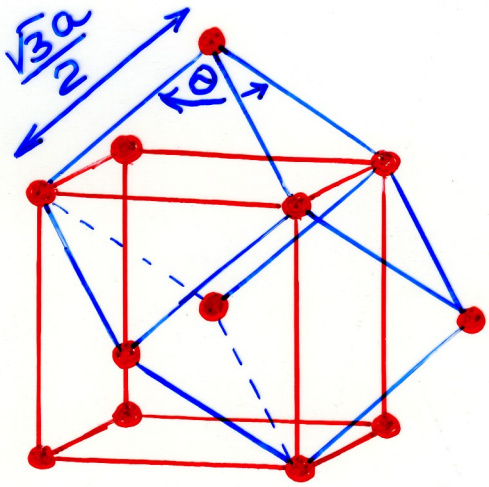
(Monatomic) Body-Centered Cubic (BCC)

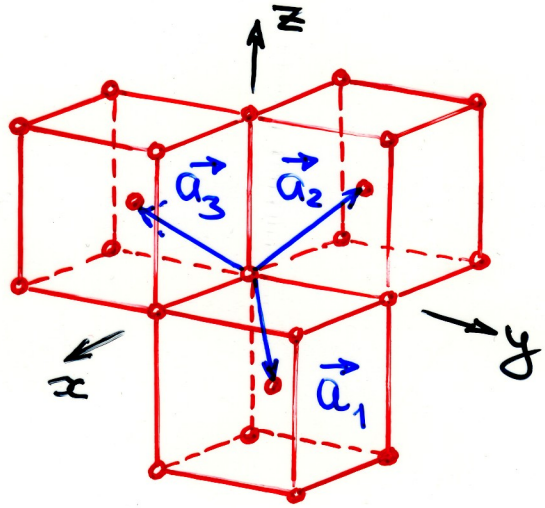
W, V, Tl, Ba, Cr, Cs, K, Li, ...



coordination number 8

nearest-neighbor distance $\frac{\sqrt{3}a}{2}$





Primitive cell

Rombohedron

$\theta = 109°28'$

Primitive vectors

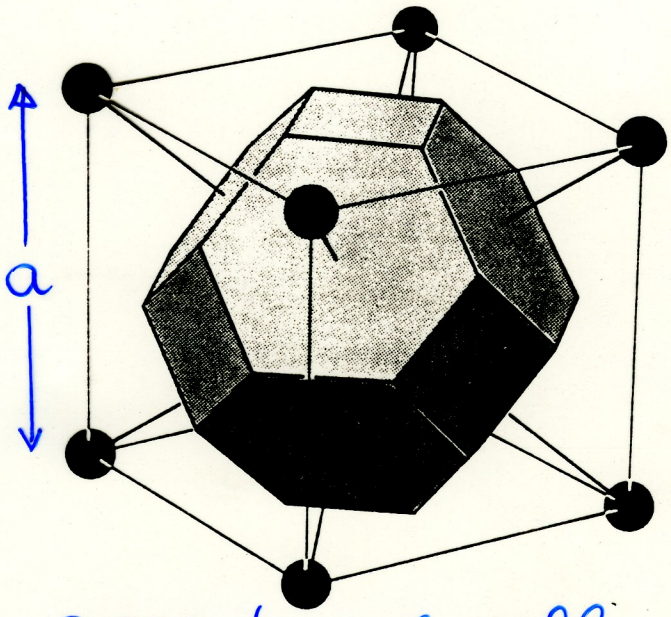
$\vec{a}_1 = \frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$

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

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

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

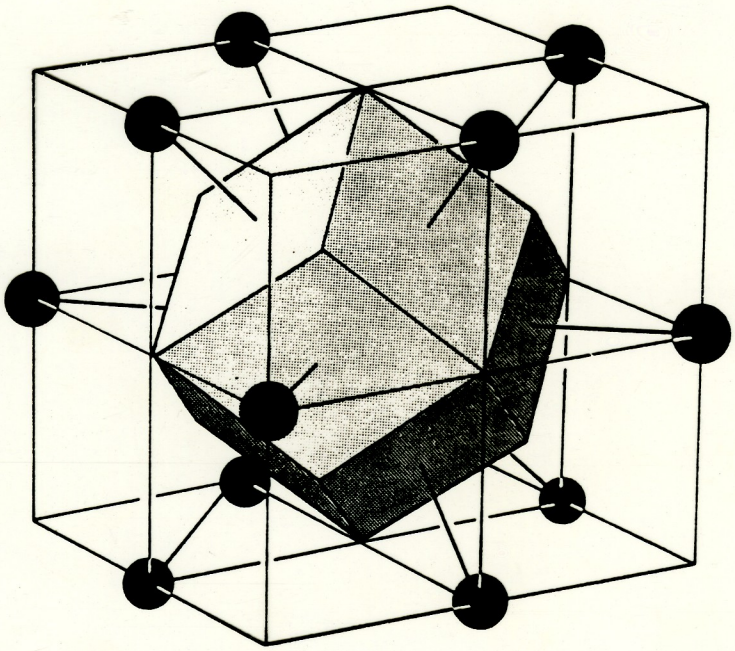
Wigner-Seitz Cell For



BCC

"truncated octahedron"

conventional cell



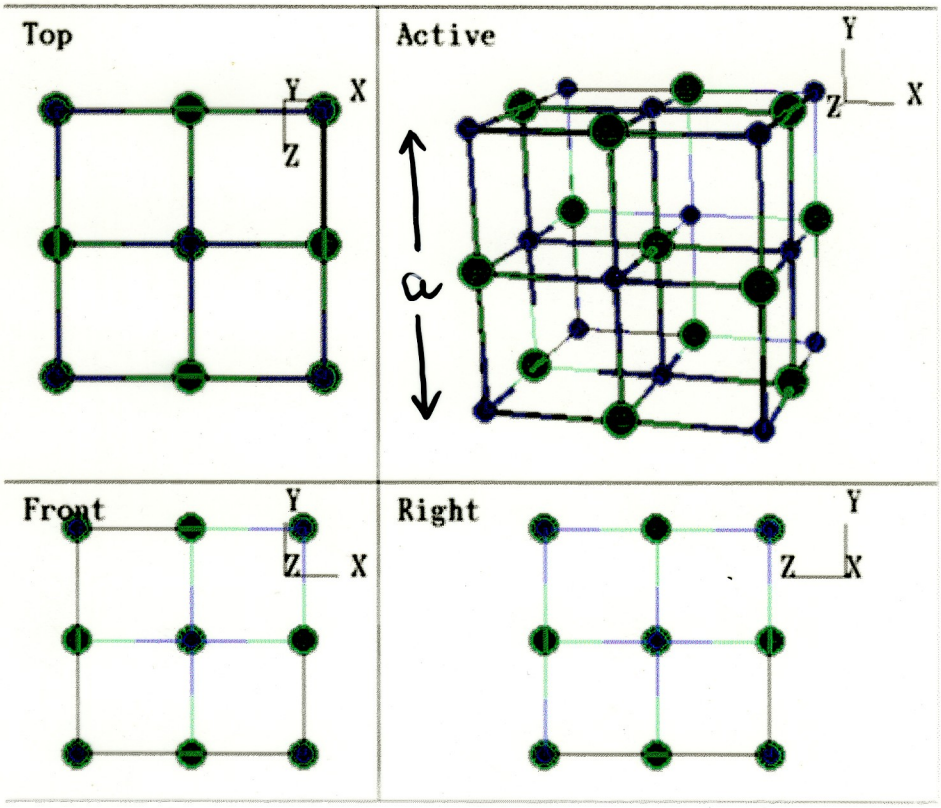
FCC

"rhombic dodecahedron"

not a conventional cell

Sodium Chloride Structure

NaCl, AgCl, CaO, KBr, ...

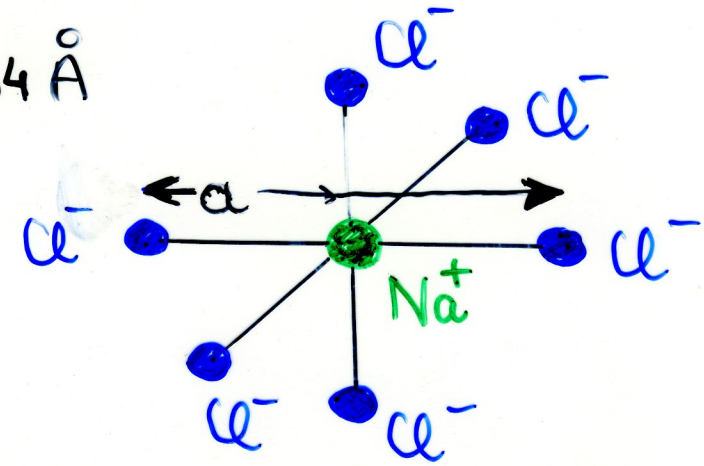


lattice constants: numbers specifying the size of a unit cell

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

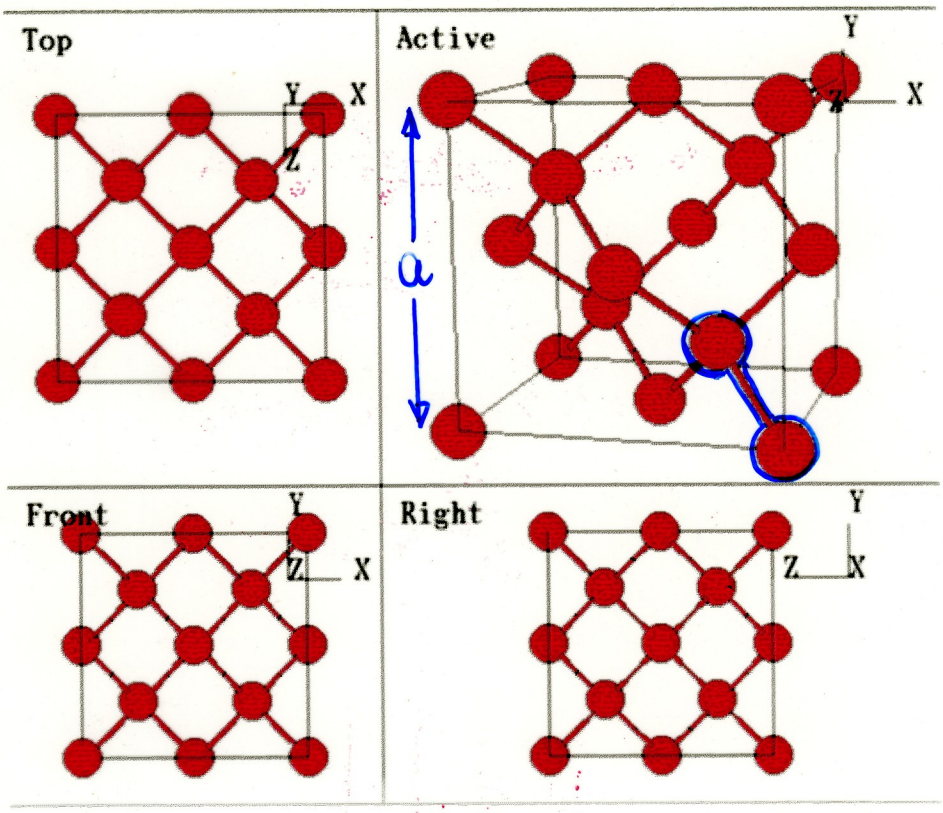


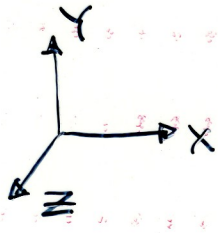
coordination number 6

18.10/ 2.8

Diamond Crystal Structure

C (diamond), Si, Ge, Sn

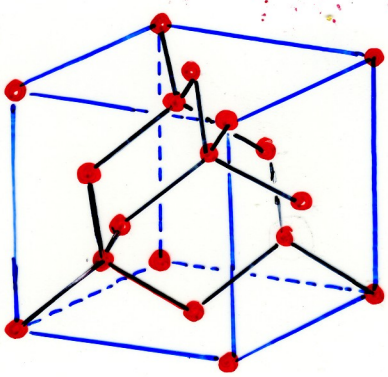




$\frac{a}{4}(-1,1,-1)$

FCC with a two-point basis

000



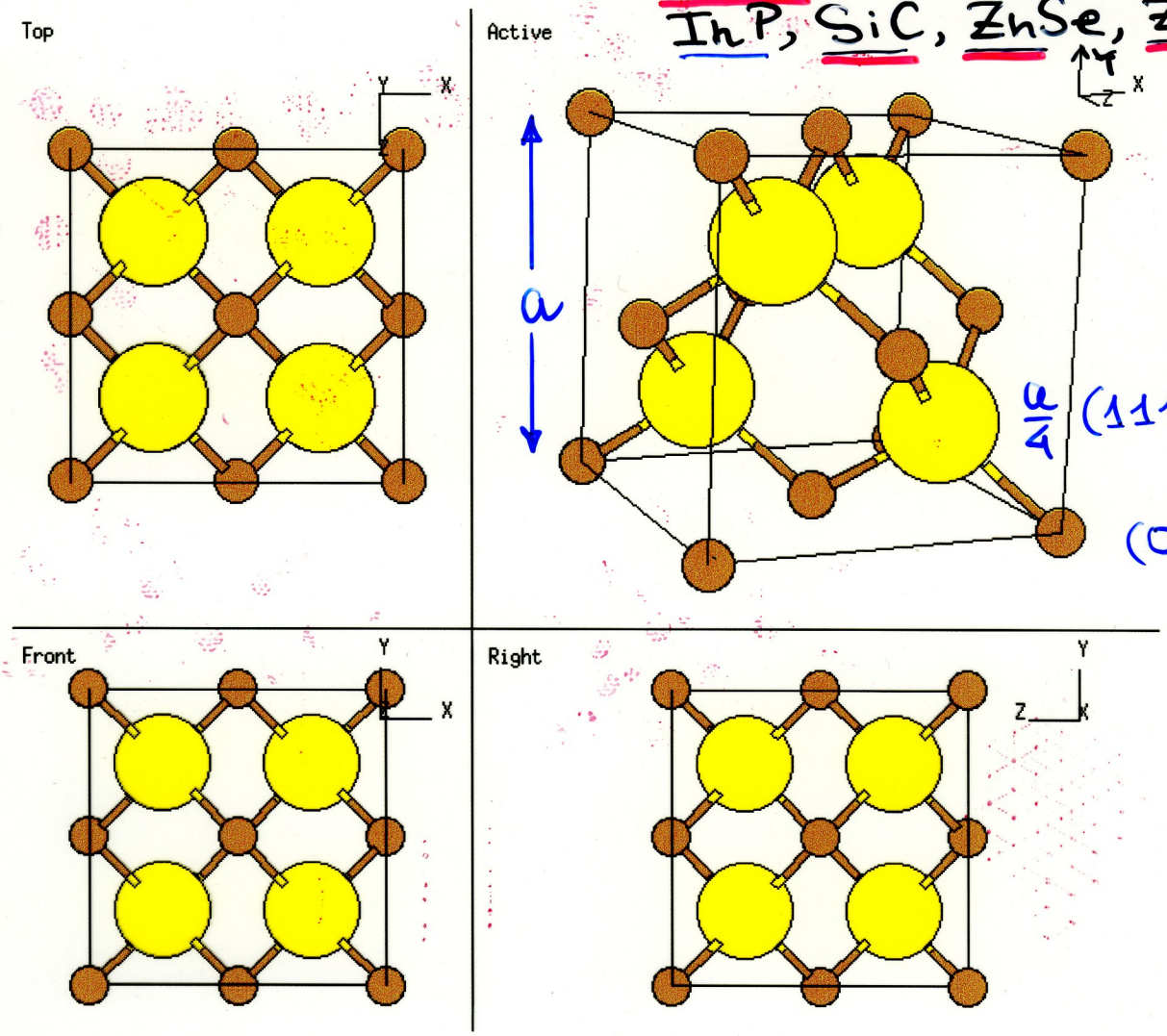
directional covalent tetrahedral bonding

coordination number 4

18.8 / 2.9

Zincblende Structure

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



Basis

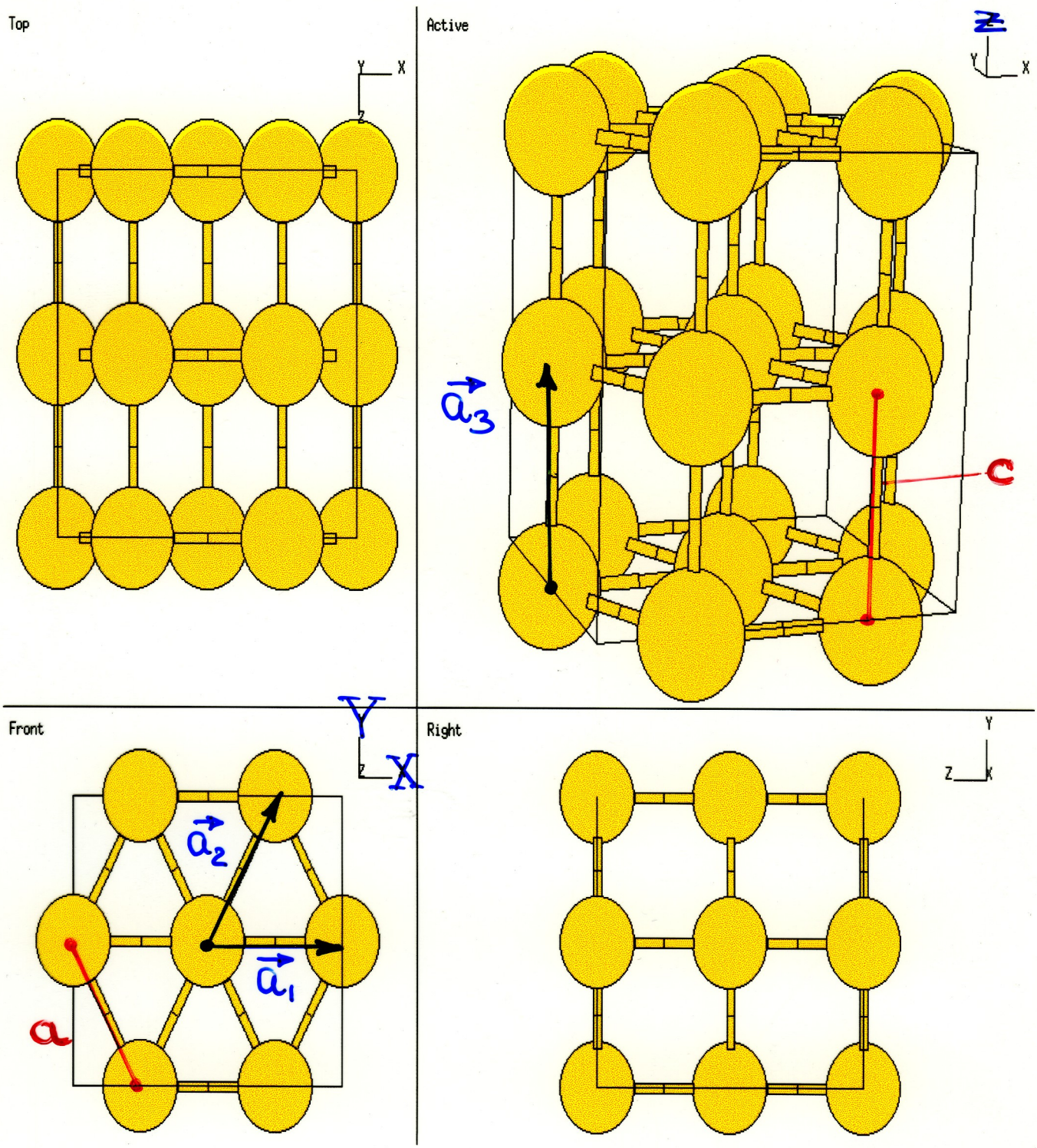
Two interpenetrating FCC lattices displaced by $\frac{1}{4}$ of the body diagonal

All III-V compound S.C.

Some II-VI compound S.C

18.9 / 210

Simple hexagonal BL (no elements in the ground state)

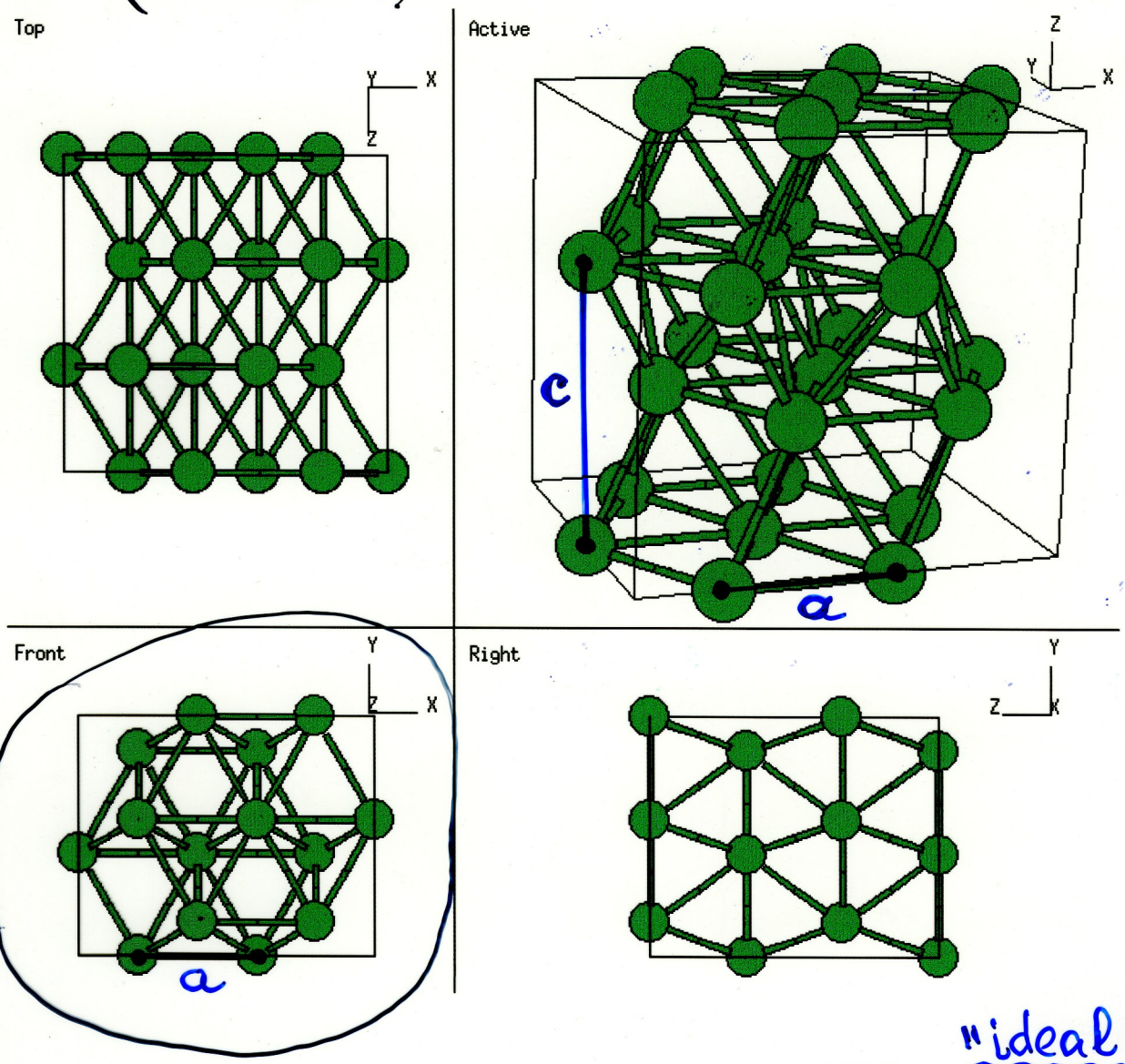


$$\vec{a}_1 = a\hat{x} \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y} \qquad \vec{a}_3 = c\hat{z}$$

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

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

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



"ideal HCP"

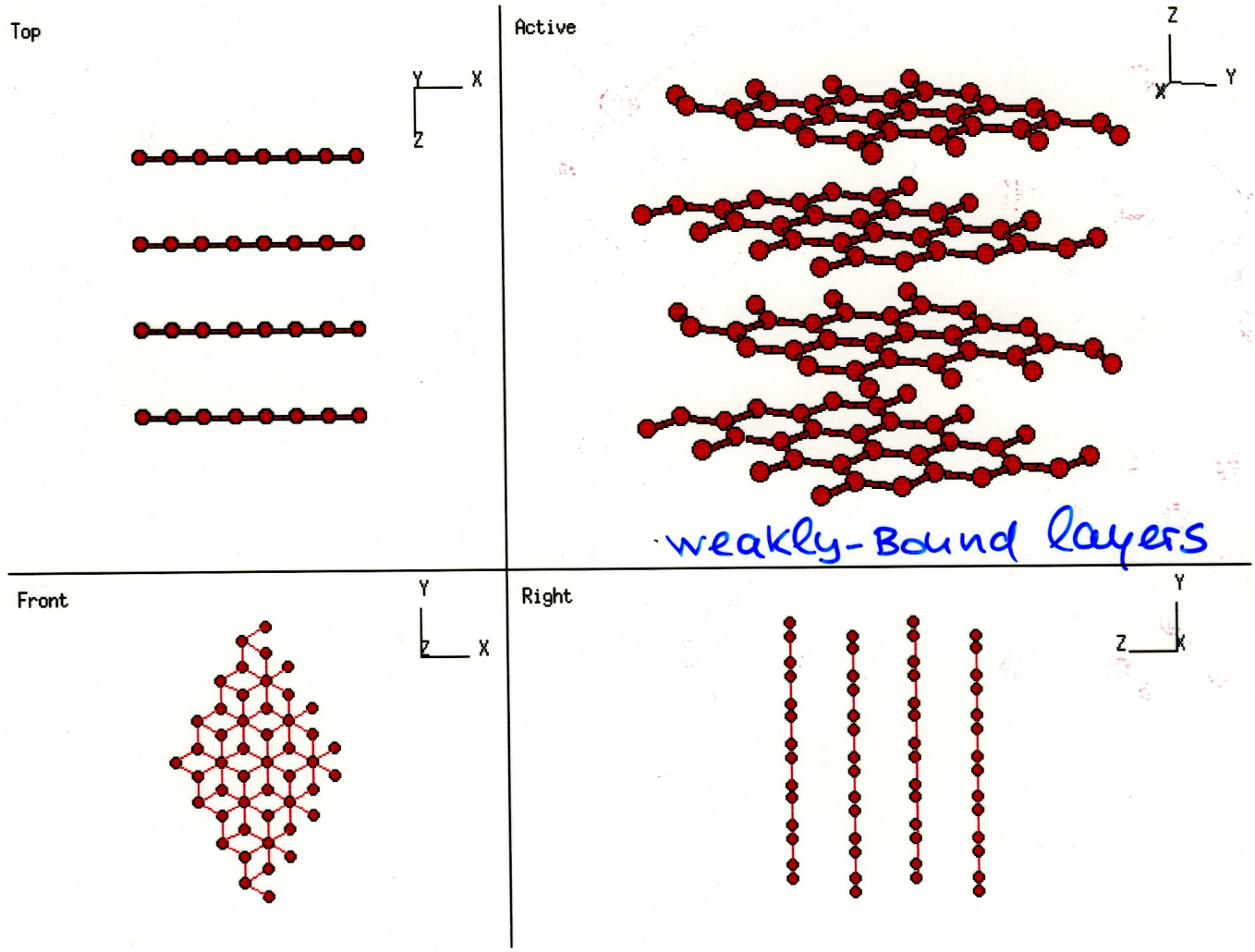
Close-packed when $c = \sqrt{\frac{8}{3}}\, a \simeq 1.63\, a$

Two interpenetrating simple hexagonal BLs

Two types of planes merge to form the 2D honeycomb

Graphite Crystal Structure

C (graphite)



weakly-Bound layers

Nobel Prize 2010

2D <u>Graphene</u>

three-connected

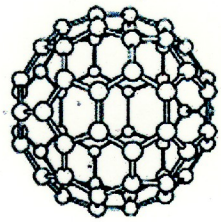
"sp^2 carbons" : one double and two single Bonds

hexagons

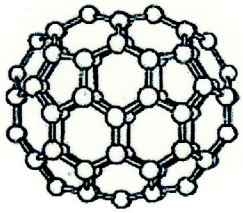
planar structure cannot be closed having only hexagons

Fullerenes

C60

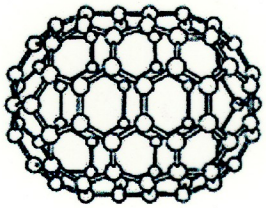


C70

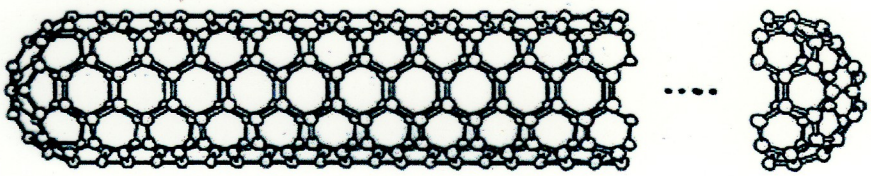


other stable hollow structures

C80 isomer



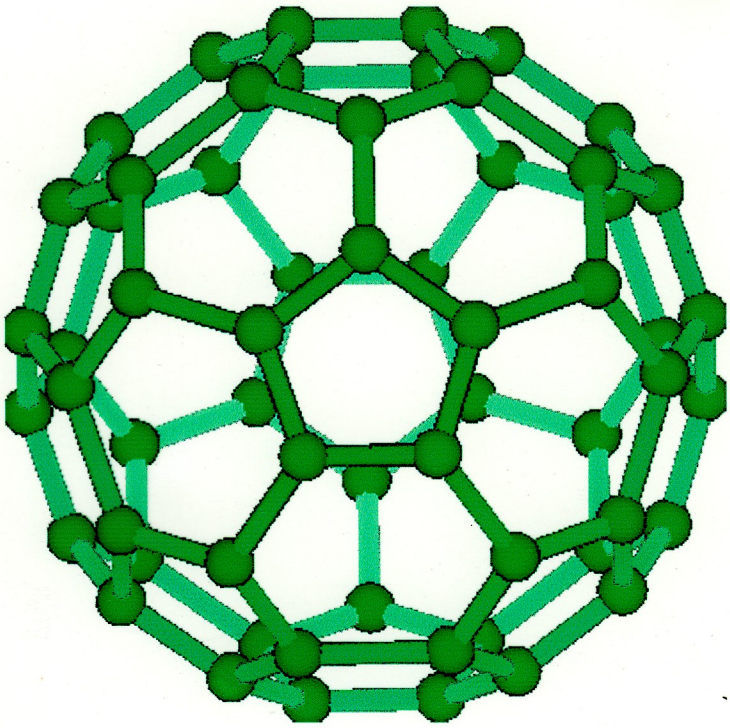
nanotube



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

- 1D physics
- metallic contacts between wires etc.

2.14



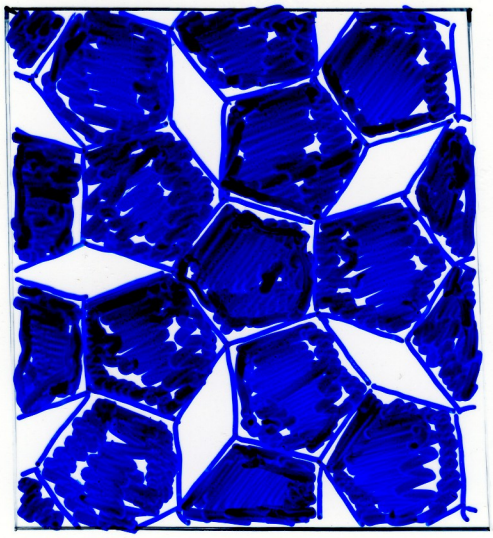
C_{60} "Fulleren"

interesting symmetries possible on a sphere!

hexagons + pentagons

$\forall$ number 12 for closure

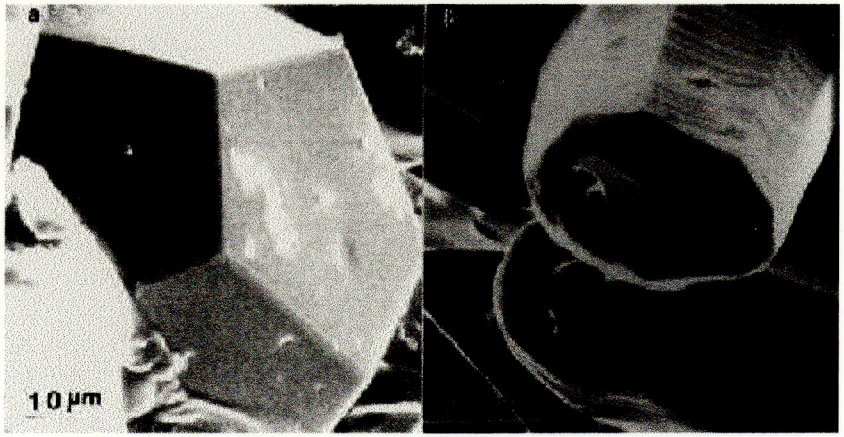
Nobel Prize in Chemistry 1996



a lattice with a fivefold axis is <u>not</u> possible on a plane:

rotations $\frac{2\pi}{5}$ and translations are not compatible

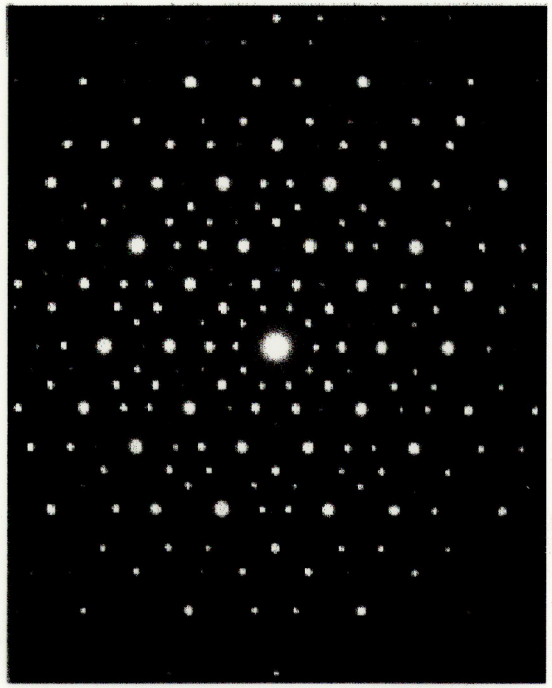
2.15



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*

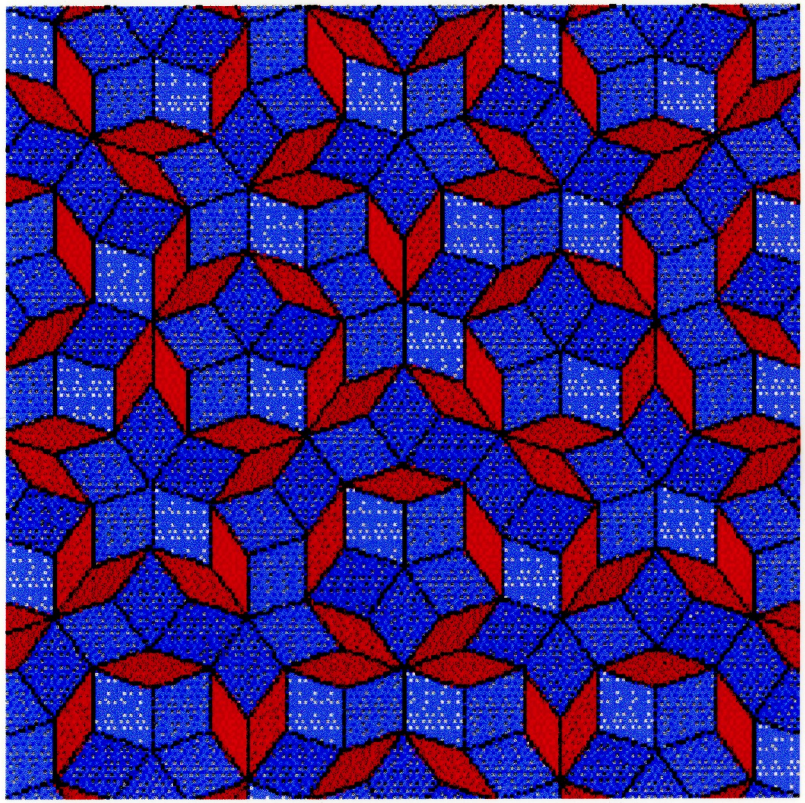


Typical diffraction diagram of a quasicrystal, exhibiting 5-fold or 10-fold rotational symmetry.

Dan Shechtman (1982)

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

Important examples

① Simple cubic BL

$$\vec{a}_1 = a\hat{x} \qquad \vec{a}_2 = a\hat{y} \qquad \vec{a}_3 = a\hat{z}$$

$$v = \left|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right| = a^3$$

$$v_B = \frac{(2\pi)^3}{v} = \frac{(2\pi)^3}{a^3}$$

$$\vec{b}_1 = \frac{2\pi}{v}\,\vec{a}_2 \times \vec{a}_3 = \frac{2\pi}{v}\,a^2\,\hat{y}\times\hat{z} = \frac{2\pi}{a}\,\hat{x}$$

$$\vec{b}_2 = \frac{2\pi}{v}\,\vec{a}_3 \times \vec{a}_1 = \frac{2\pi}{v}\,a^2\,\hat{z}\times\hat{x} = \frac{2\pi}{a}\,\hat{y}$$

$$\vec{b}_3 = \frac{2\pi}{v}\,\vec{a}_1 \times \vec{a}_2 = \frac{2\pi}{v}\,a^2\,\hat{x}\times\hat{y} = \frac{2\pi}{a}\,\hat{z}$$

Simple cubic with lattice constant a

$$v = a^3$$

Reciprocal simple cubic with latt. const. $\frac{2\pi}{a}$

$$v_B = \left(\frac{2\pi}{a}\right)^3 = \frac{(2\pi)^3}{v}$$

Direction of $\vec{A}\times\vec{B}$?

The rule of the RIGHT leg:

$$(\vec{A}\times\vec{B})\cdot\vec{C} > 0$$

II. Face-centered cubic BL (FCC) $v = a^3/4$

$$\vec{a}_1 = \frac{1}{2}a(\hat{x}+\hat{y}) \quad \vec{a}_2 = \frac{1}{2}a(\hat{x}+\hat{z}) \quad \vec{a}_3 = \frac{1}{2}(\hat{y}+\hat{z})$$

RL: $$\vec{b}_1 = \frac{2\pi}{v}\cdot(\vec{a}_2\times\vec{a}_3) = \frac{2\pi}{v}\cdot\frac{a^2}{4}\cdot(\hat{x}+\hat{z})\times(\hat{y}+\hat{z})$$

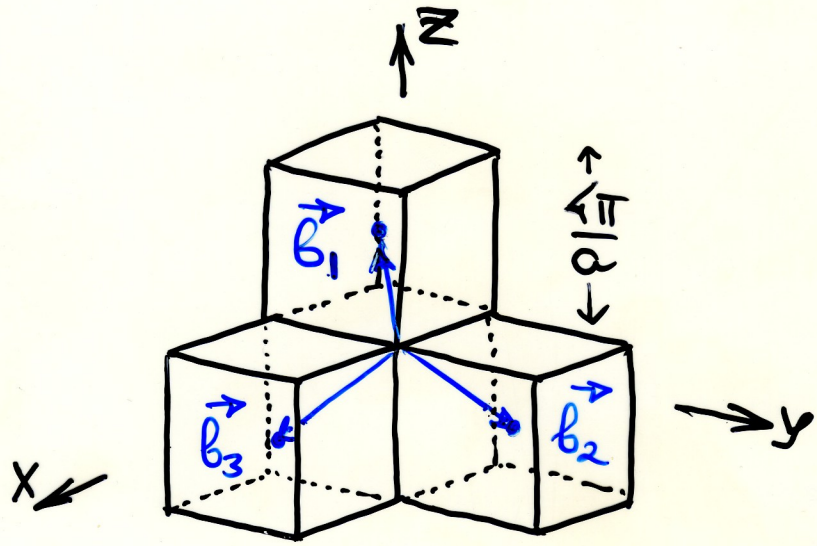
✓ $$\vec{b}_1 = \frac{2\pi}{a}(\hat{z}-\hat{y}-\hat{x}) = \underline{\frac{4\pi}{a}\cdot\frac{1}{2}(-\hat{x}-\hat{y}+\hat{z})}$$

$$\vec{b}_2 = \frac{2\pi}{v}\vec{a}_3\times\vec{a}_1 = \frac{2\pi}{v}\cdot\frac{a^2}{4}\cdot(\hat{y}+\hat{z})\times(\hat{x}+\hat{y})$$

✓ $$\vec{b}_2 = \frac{2\pi}{a}(-\hat{z}+\hat{y}-\hat{x}) = \underline{\frac{4\pi}{a}\cdot\frac{1}{2}(-\hat{x}+\hat{y}-\hat{z})}$$

$$\vec{b}_3 = \frac{2\pi}{v}\vec{a}_1\times\vec{a}_2 = \frac{2\pi}{v}\cdot\frac{a^2}{4}\cdot(\hat{x}+\hat{y})\times(\hat{x}+\hat{z})$$

✓ $$\vec{b}_3 = \frac{2\pi}{a}(-\hat{y}-\hat{z}+\hat{x}) = \underline{\frac{4\pi}{a}\,\frac{1}{2}(\hat{x}-\hat{y}-\hat{z})}$$



BCC primitive vectors!

BL		RL
SC (a)	$\longrightarrow$	SC $\left(\frac{2\pi}{a}\right)$
FCC (a)	$\longrightarrow$	BCC $\left(\frac{4\pi}{a}\right)$
BCC (a)	$\longrightarrow$	FCC $\left(\frac{4\pi}{a}\right)$
simple hexagonal (a, c)	$\longrightarrow$	simple hexagonal $\left(\frac{4\pi}{\sqrt{3}a}, \frac{2\pi}{c}\right)$

First Brillouin Zone

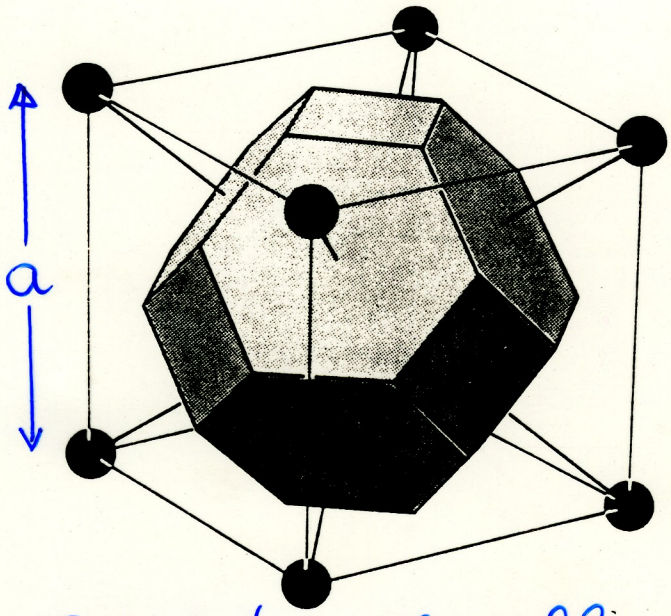
is the Wigner-Seitz cell of the reciprocal lattice

Direct lattice : $\vec{r}$ - space (coordinates)

Reciprocal lattice : $\vec{k}$ - space (wave vectors)

First Brillouin Zone is just some region in $\vec{k}$ - space

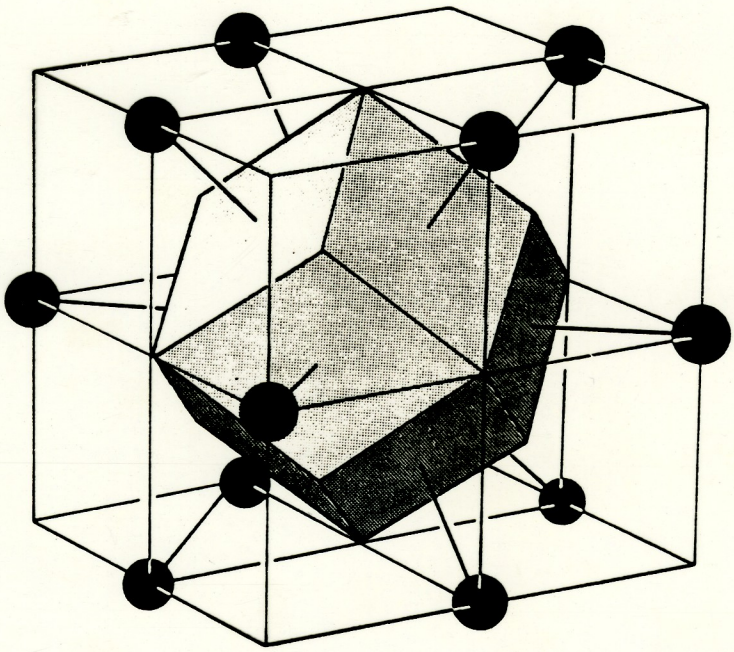
Wigner-Seitz Cell For



BCC

"truncated octahedron"

conventional cell



FCC

"rhombic dodecahedron"

not a conventional cell