Introduction to Solid State Physics

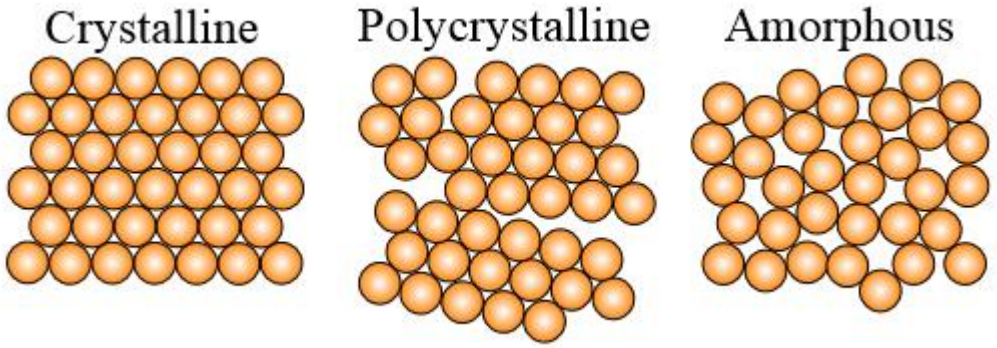
or the study of physical properties of matter in a solid phase

Prof. Germar Hoffmann

1. Crystal Structures
2. Reciprocal Lattice
3. Crystal Binding and Elastic Constants
4. Phonons I. Crystal Vibrations

Prof. Raynien Kwo

5. Phonons II. Thermal Properties
6. Free Electron Fermi Gas
7. Energy Bands
8. Semiconductor Crystals



A: Material	B: Structure	C: Shape	D: Properties
metal semiconductor insulator *superconductors* *magnetism* *topological insulators*	crystalline amorphous quasicrystal	bulk surface interface nanocluster	electrical optical thermal mechanical ....

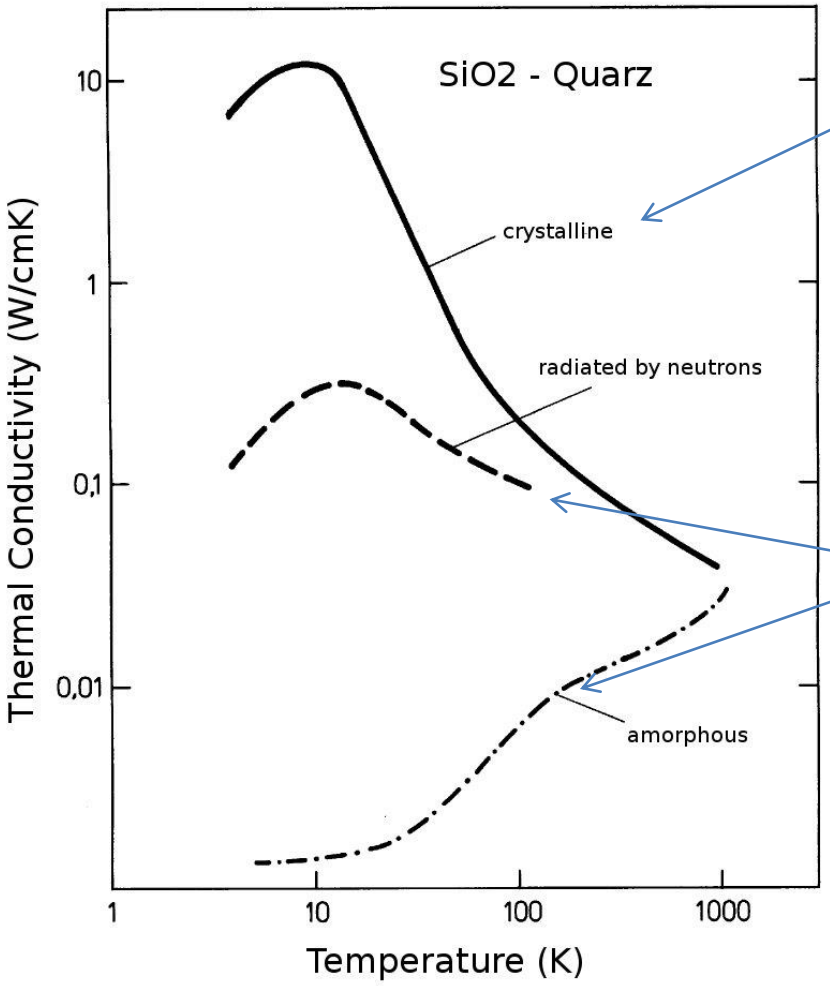
Solid State Physics = {A} X {B} X {C} X {D}

Thermal Conductivity of SiO_2: $Q = \lambda \nabla T$

Q : Thermal Current Density

λ: coefficient of Thermal Conductivity

∇T: Temperature Gradient



can be theoretically understood

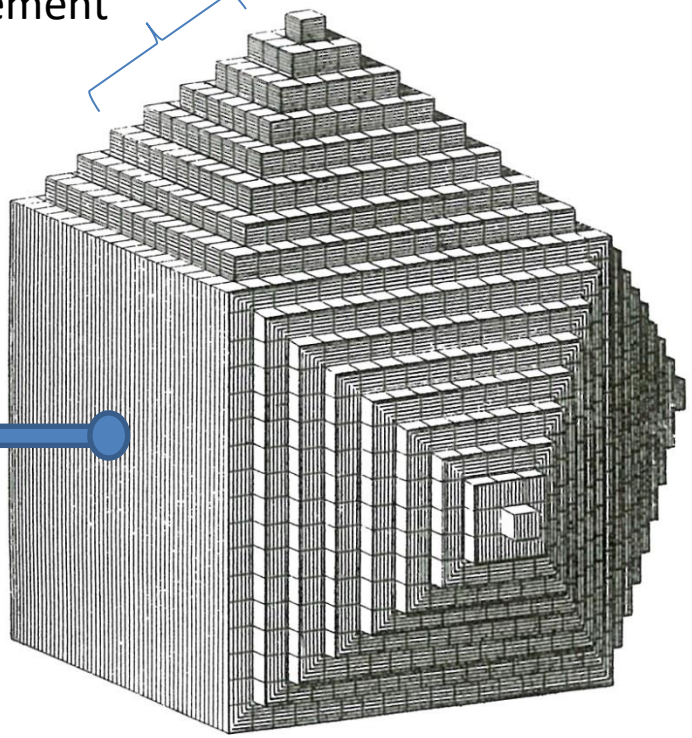
Condensed Matter Physics

complicated

Condensed Matter Physics

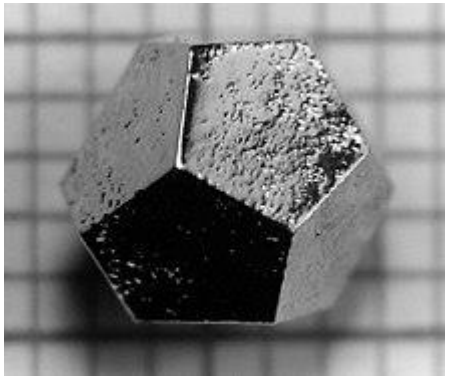
Unit Cell
(one or more atoms)

Periodic Arrangement



(a)

crystal planes



=> quasicrystal (NP 2011 Dan Shechtman)

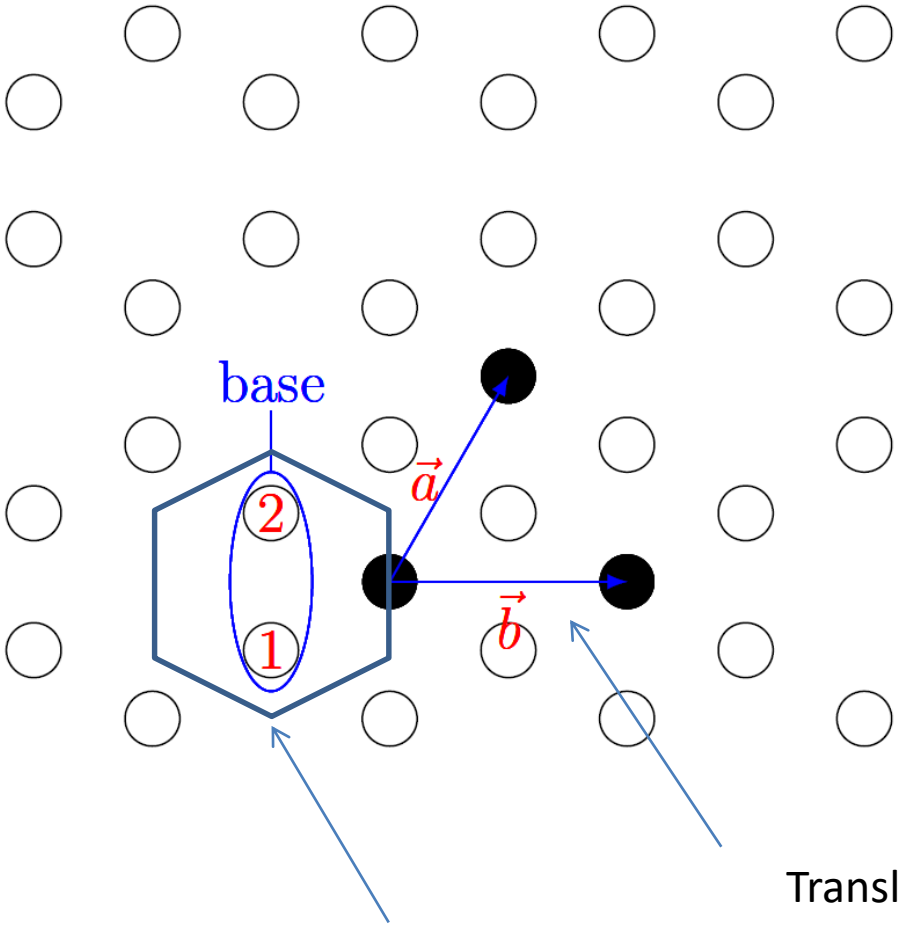
- Crystal Structure
  - Lattice + Basis
  - Symmetry Operations
  - Wigner Seitz Cell
  - Lattice Planes

- Experimental Methods

Crystal Structure in 2 Dimensions

atoms

periodic arrangement of atoms / unit cells



Translation Vectors **a,b,c**

r' = **r** + u_1**a** + u_2**b** + u_3**c**

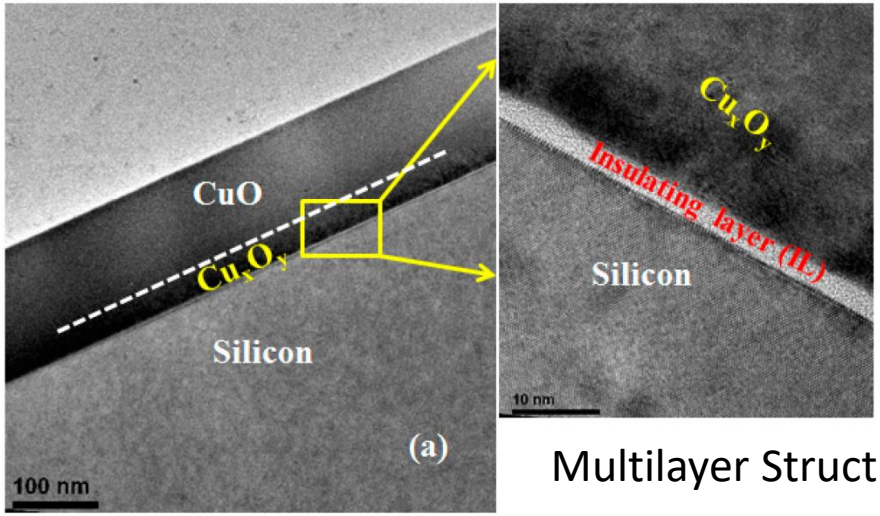
u_1, u_2, u_3: arbitrary integer

set of points **r'** for all u_1, u_2, u_3 defines a lattice

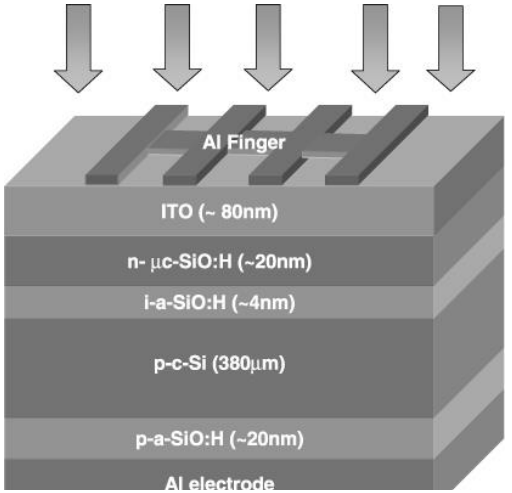
Translational Vectors

Unit Cell (group of atoms)

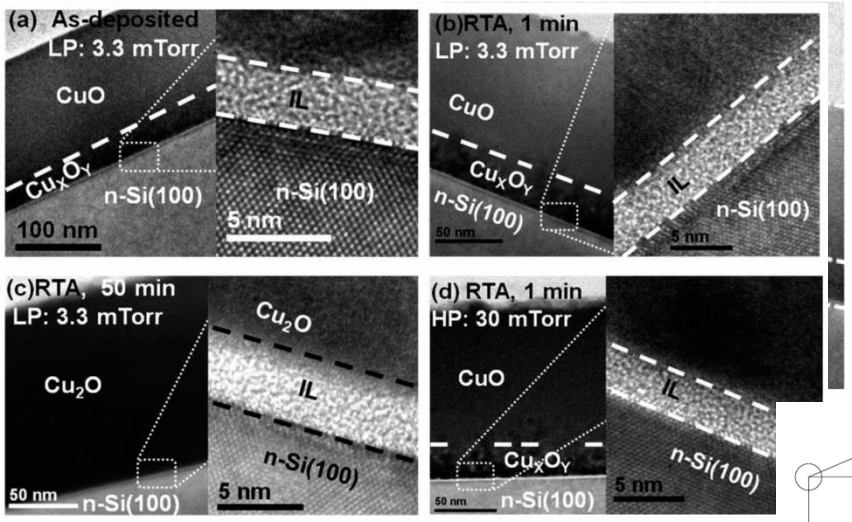
TEM



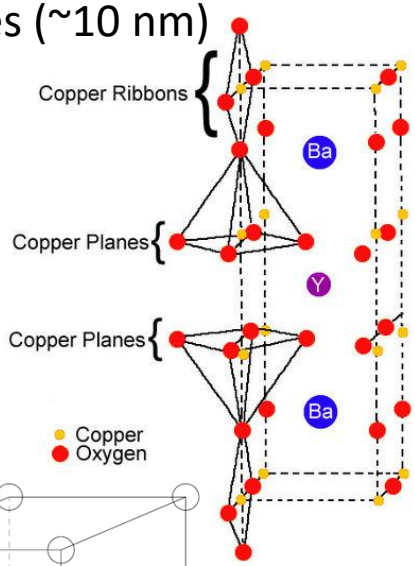
Solar Cell



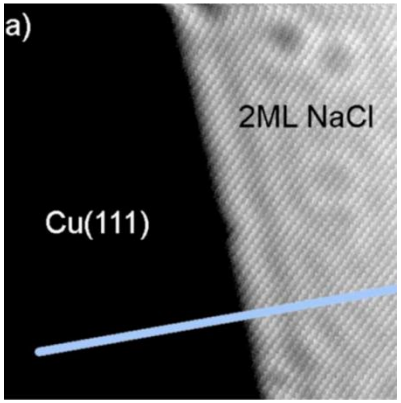
Multilayer Structures (~10 nm)



TKS. Wong et al., Materials 9. 271 (2016)

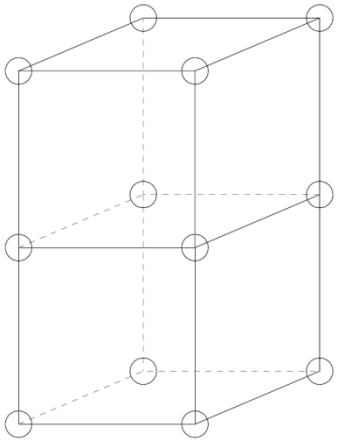


Layered Structure (~nm)
Here: YBCO
(superconductor)



STM

Atomic Structure (~Å)



UNIT CELLS:

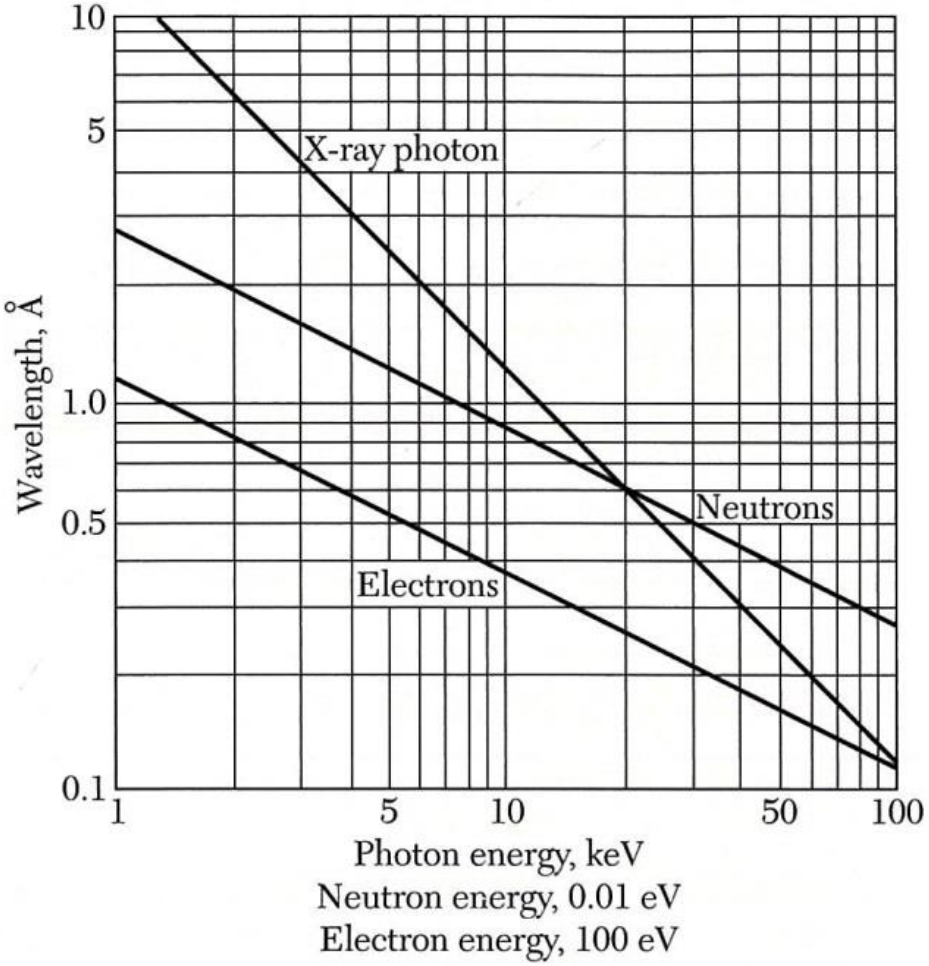
Study of Structures

$\lambda = hc / E$

h = Planck constant

c = speed of light

E = Photon Energy



Volume / Surface Averaging Techniques

- x-ray diffraction
- neutron diffraction
- electron diffraction

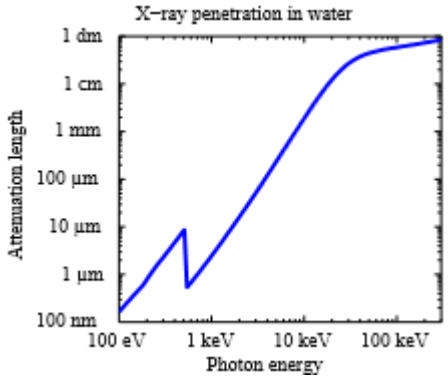
$\lambda = h / (mv)$

m = particle mass

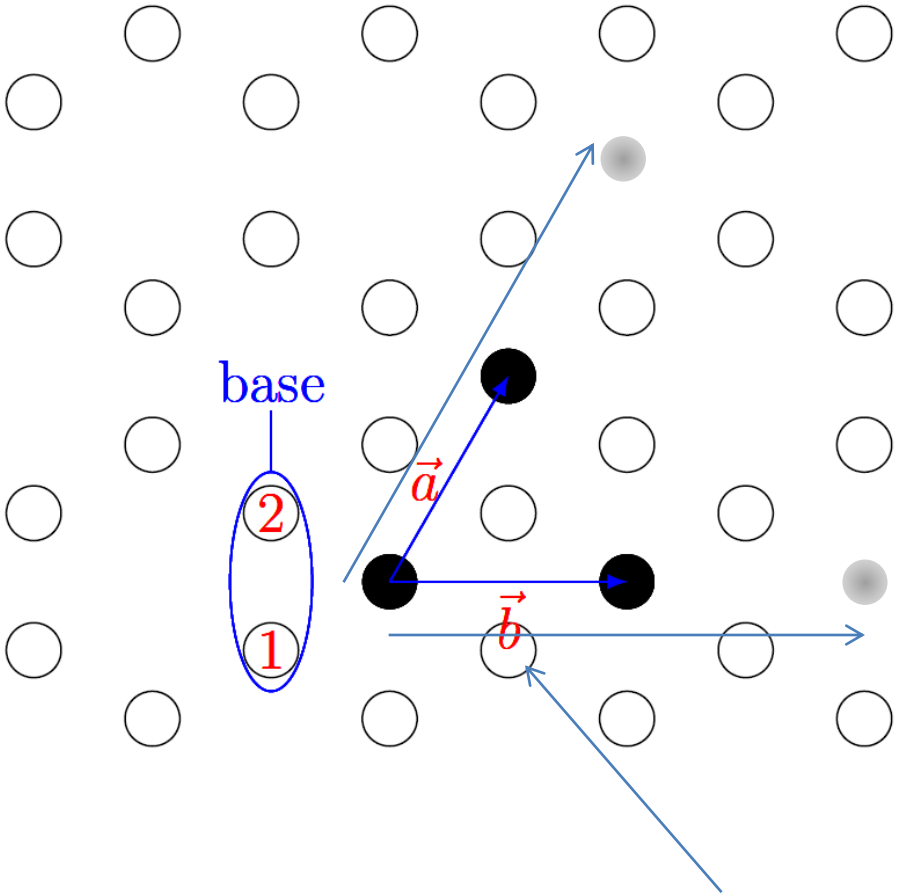
v = particle speed

Surface Sensitive Techniques

- Scanning Probe Microscopy
  - Scanning Tunneling Microscopy (STM)
  - Atomic Force Microscopy (AFM)
  - Kelvin Probe Microscopy (KPM)



Primitive Translation Vectors



Translation Vectors **a,b,c**

$\mathbf{r'} = \mathbf{r} + u_1\mathbf{a} + u_2\mathbf{b} + u_3\mathbf{c}$

u_1, u_2, u_3: arbitrary integer

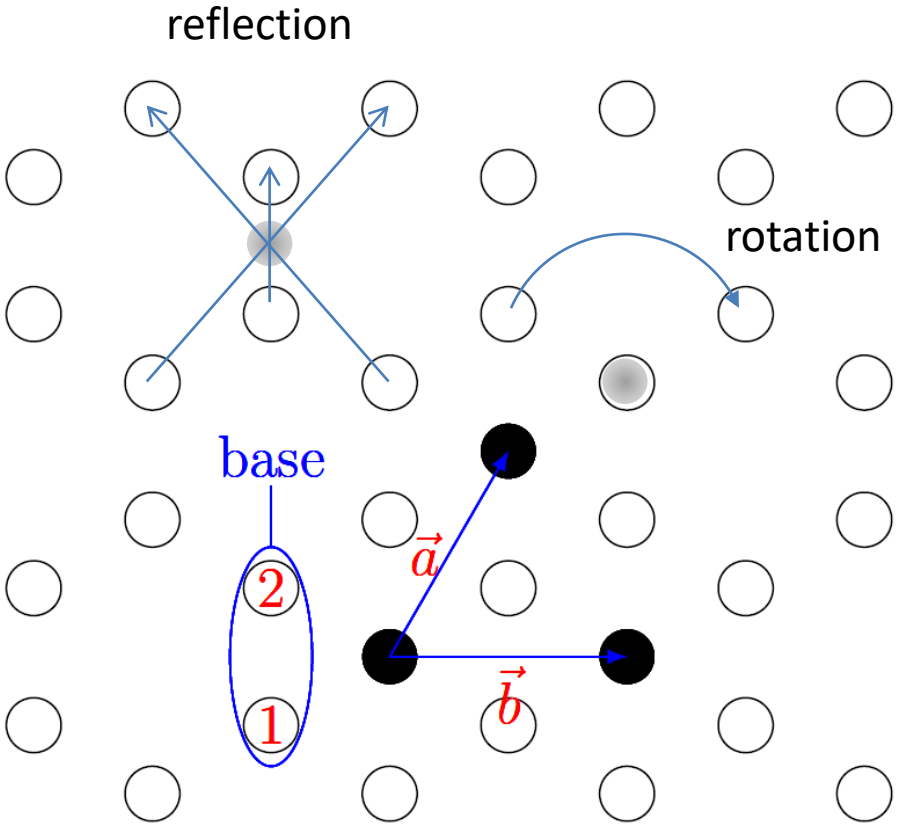
set of points **r'** for all u_1, u_2, u_3 defines a lattice

Translation Operator

$\mathbf{T} = u_1\mathbf{a} + u_2\mathbf{b} + u_3\mathbf{c}$

smallest translation vectors
= primitive translation vectors

Symmetry Operation



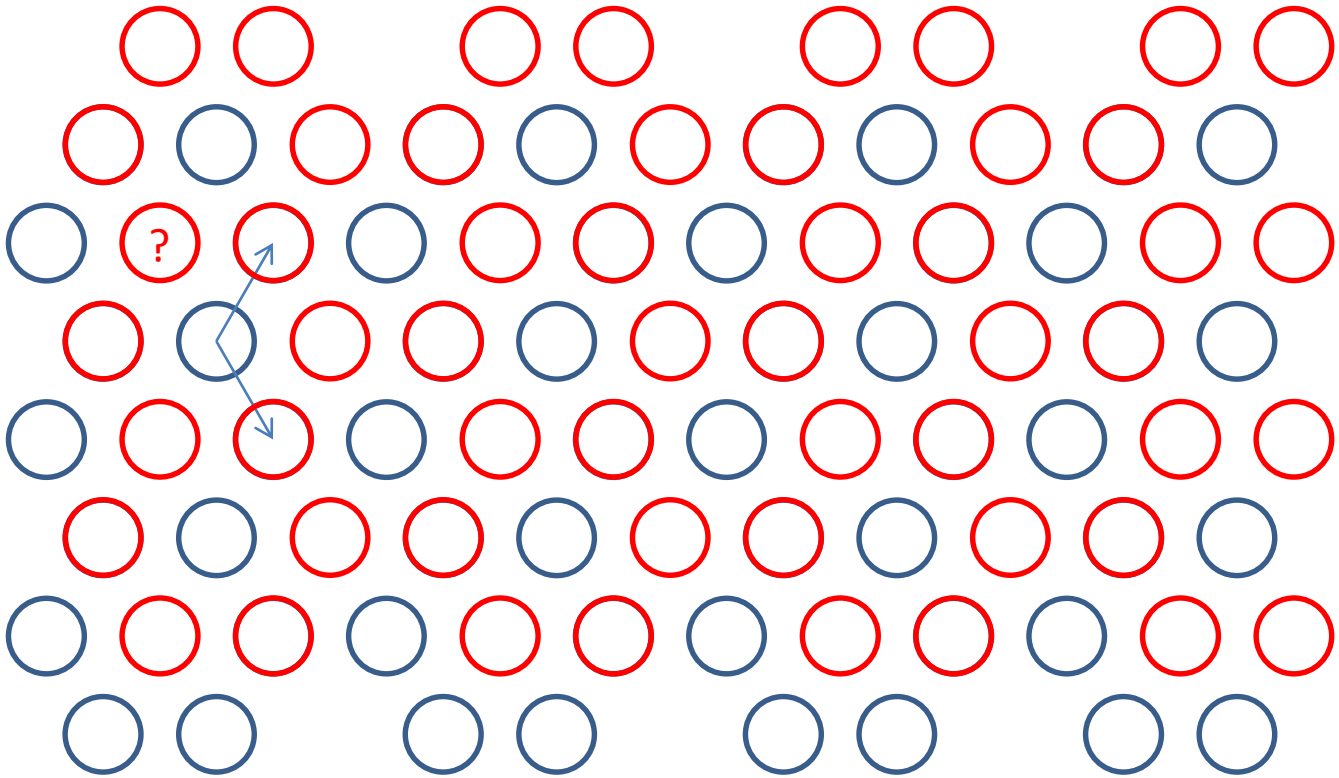
Translation Operator

Point Operators

1. rotation
2. reflection

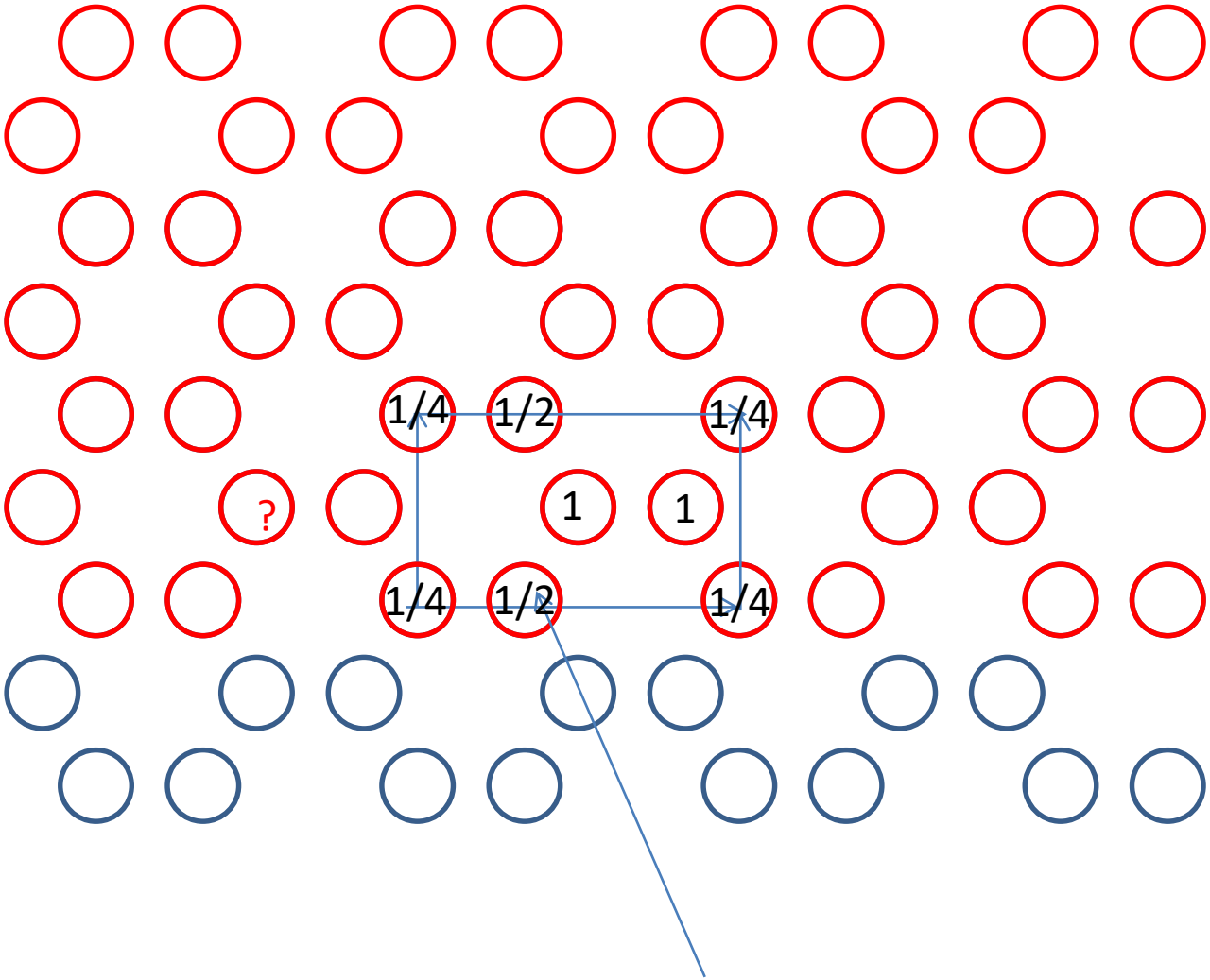
Symmetry Operations reflect the crystal structure

Translation Operator:



No ! ….. The Structure must be identical before and after translation !

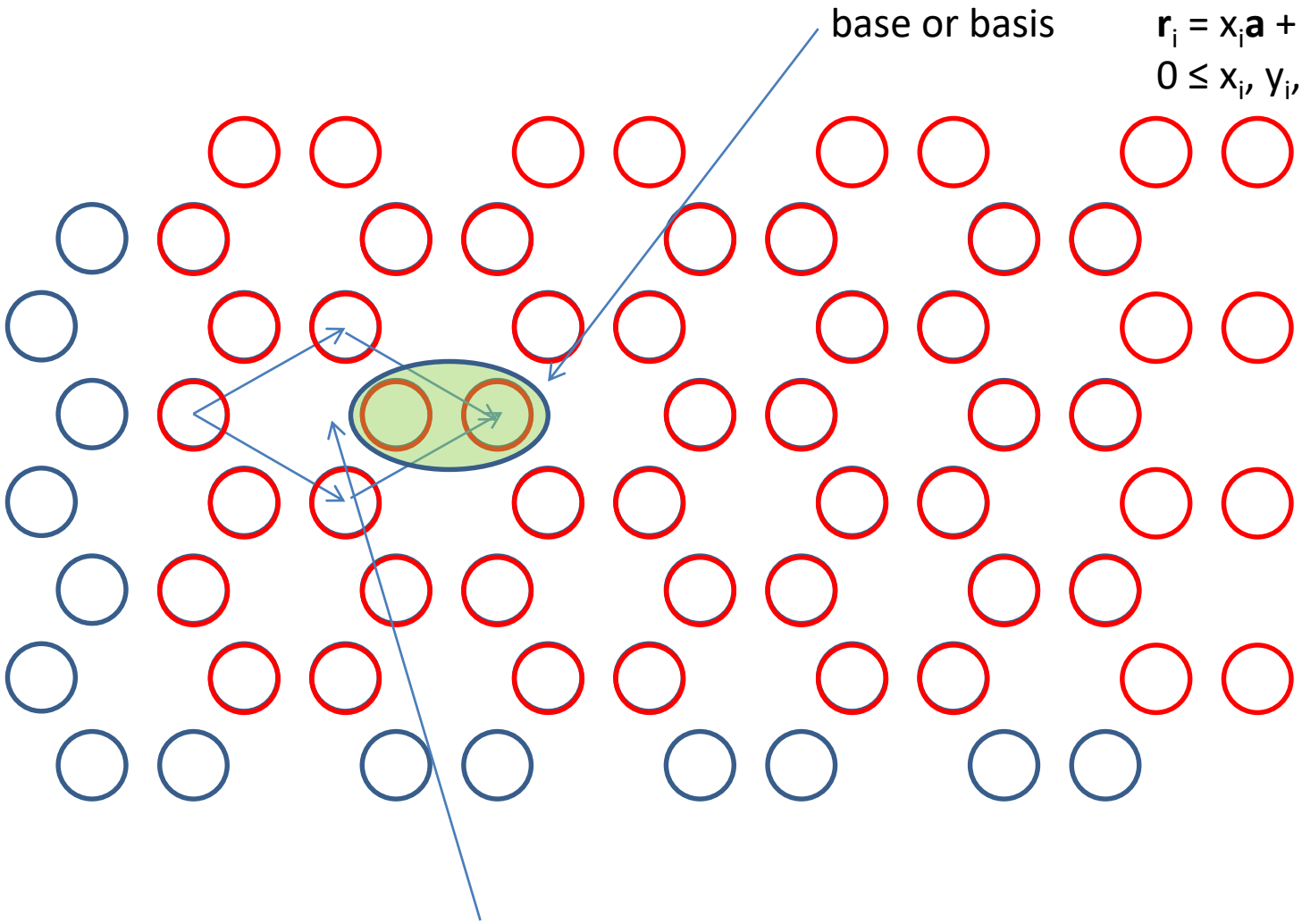
Translation Operator & Unit Cell:



Conventional Unit Cell (4 atoms)

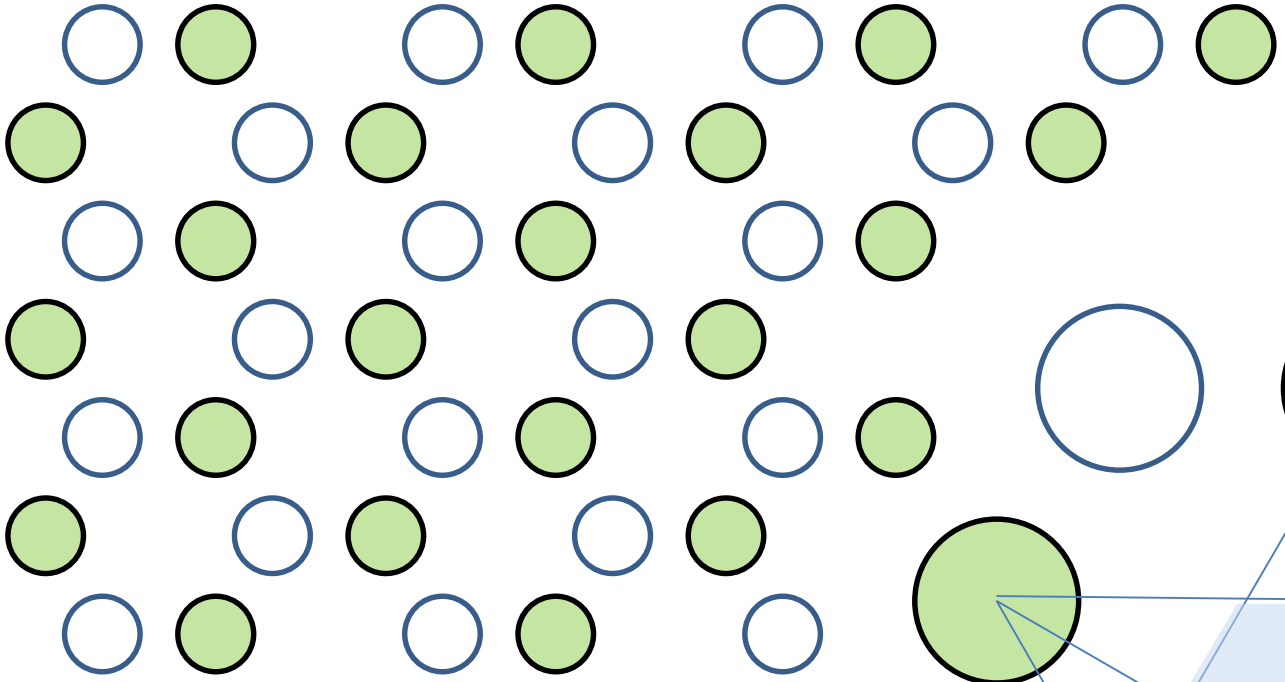
Smallest Possible Unit Cell ? – No !

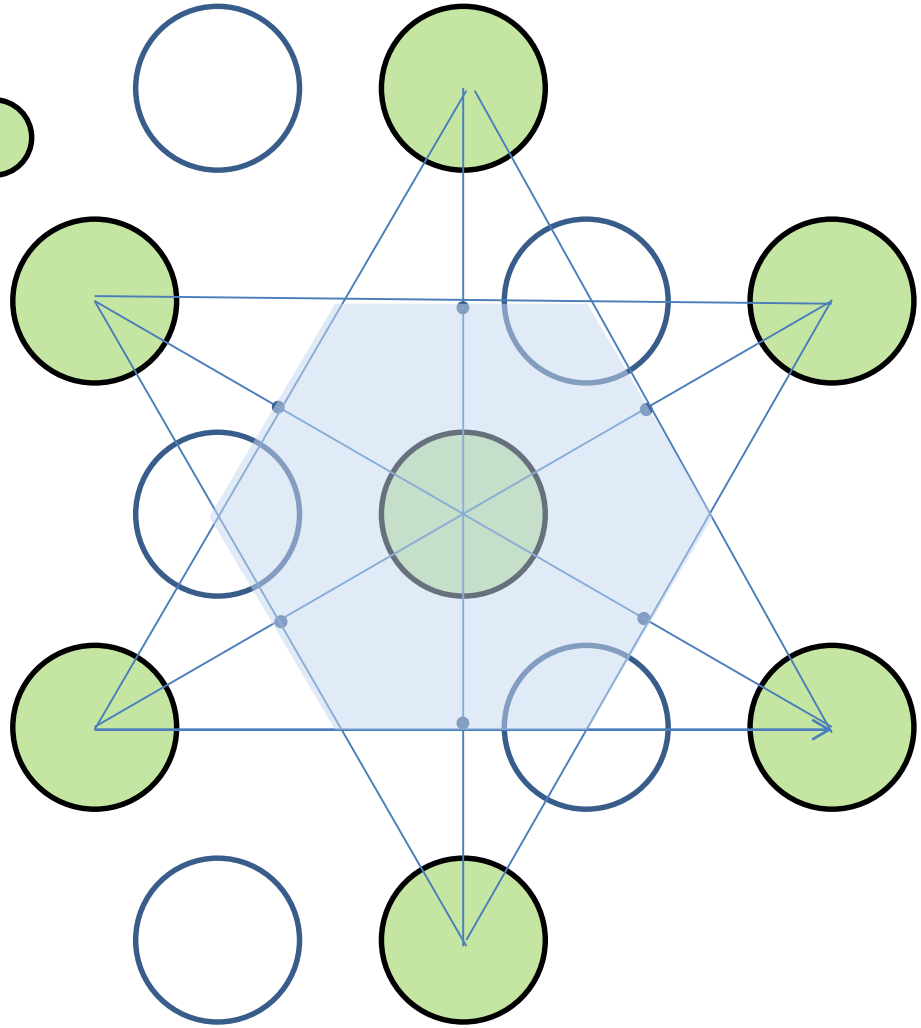
Primitive Translational Operators & Primitive Unit Cell:



Smallest possible unit cell = primitive unit cell (2 atoms)

Does the Unit Cell (u.c.) have the symmetry of the crystal ? – No !





Wigner-Seitz Cell:

Primitive Unit Cell

+

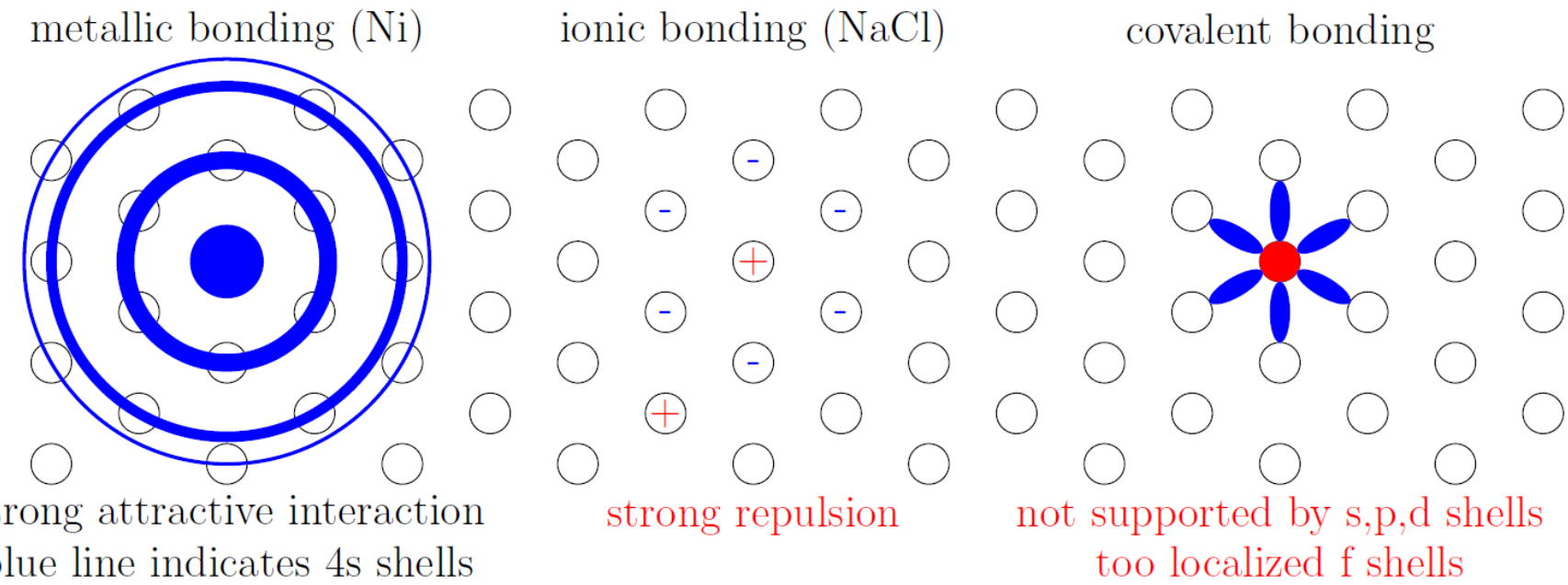
Full Crystal Symmetry

1st: Connect one atom with all neighbors

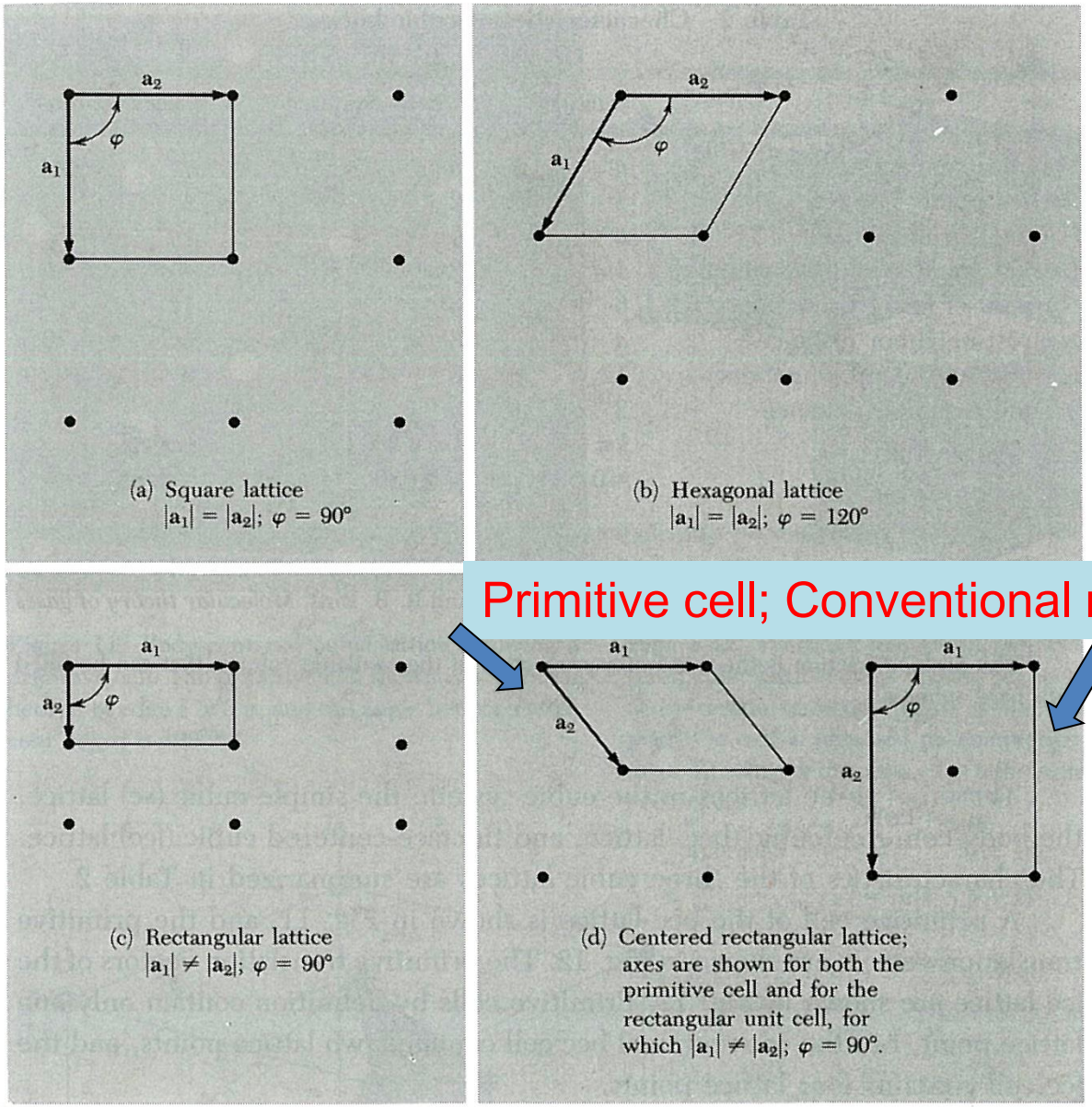
2nd: Mark Middle Point

3rd: Draw Lines through points and perpendicular to interconnecting lines

Why do we have different crystal lattices ?



Two - Dimensional lattices (1 oblique + 4 special)

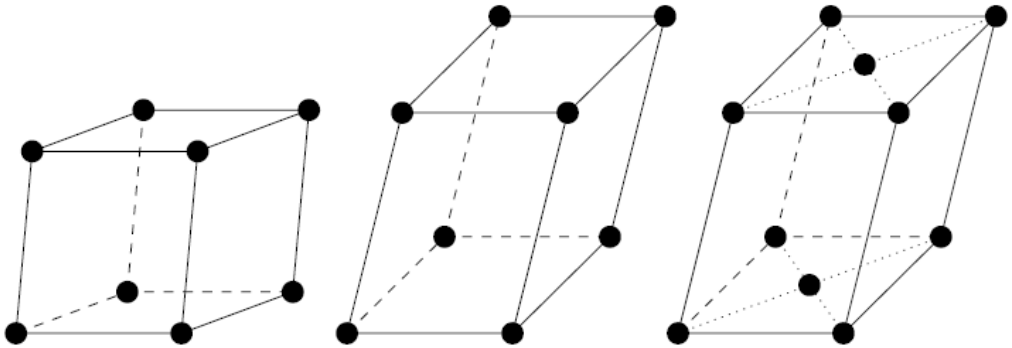


Primitive cell; Conventional rectangular cell

Figure 9 Four special lattices in two dimensions

Table 1 The 14 lattice types in three dimensions

System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$

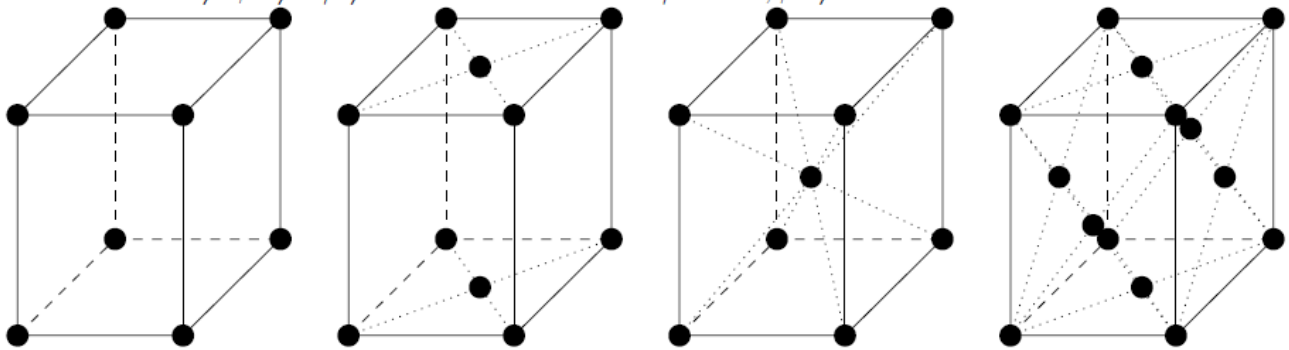


monoclinic

triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90$

primitive
$a \neq b \neq c$
$\alpha = \gamma = 90; \beta \neq 90$

base centered



orthorhombic

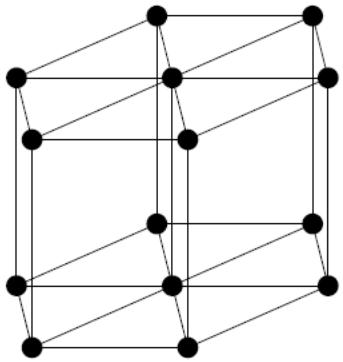
primitive

base centered

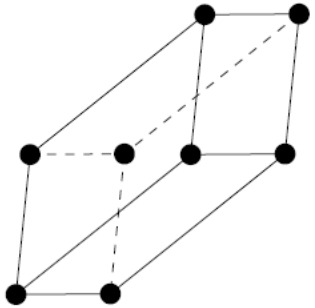
body centered

face centered

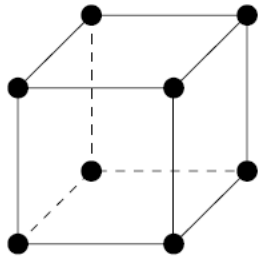
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90$

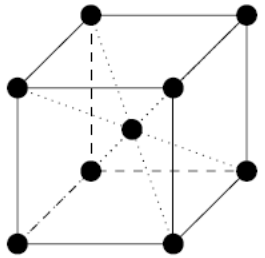


hexagonal
$a = b \neq c$
$\alpha = \beta = 90; \gamma = 120$

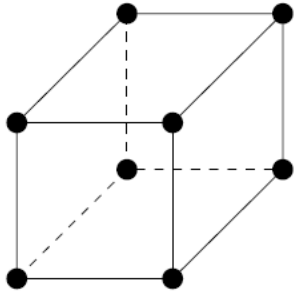


rhombic
$a = b = c$
$\alpha = \beta = \gamma \neq 90$

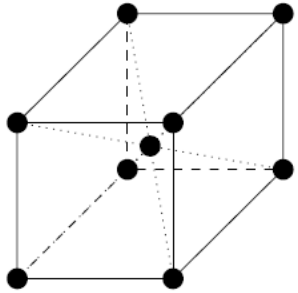




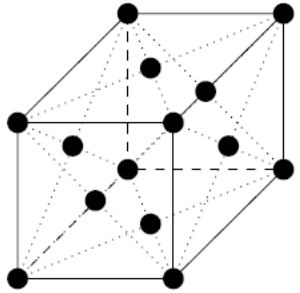
tetragonal
primitive body centered
$a = b \neq c$
$\alpha = \beta = \gamma = 90$



primitive



cubic
body centered
$a = b = c$
$\alpha = \beta = \gamma = 90$



face centered

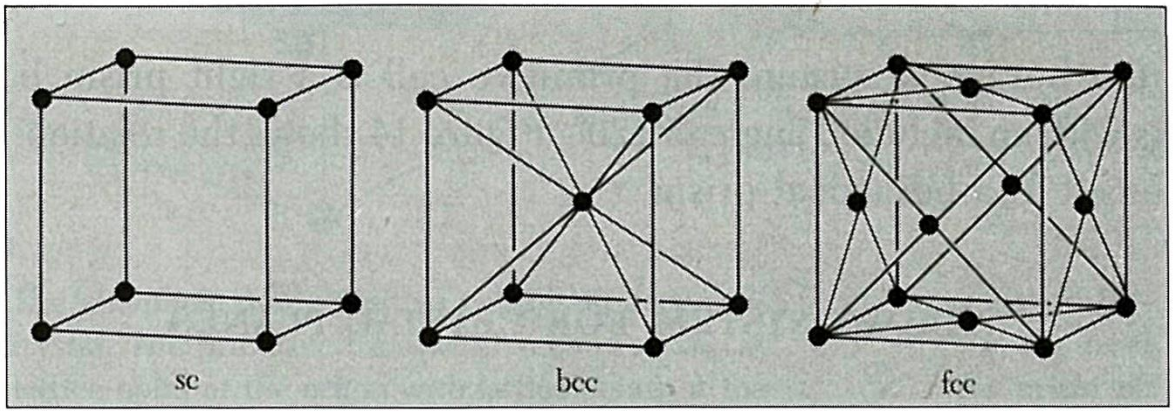


Figure 10 The cubic space lattices. The cells shown are the conventional cells.

Table 2 Characteristics of cubic lattices[a]

	Simple	Body-centered	Face-centered
Volume, conventional cell	a^3	a^3	a^3
Lattice points per cell	1	2	4
Volume, primitive cell	a^3	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors[a]	6	8	12
Nearest-neighbor distance	a	$3^{1/2}a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$2^{1/2}a$	a	a
Packing fraction[b]	$\frac{1}{6}\pi$ $= 0.524$	$\frac{1}{8}\pi\sqrt{3}$ $= 0.680$	$\frac{1}{6}\pi\sqrt{2}$ $= 0.740$

face centered cubic (fcc)

Table 4.1
ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ-Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β-Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49

Data in Tables 4.1 to 4.7 are from R. W. G. Wyckoff, *Crystal Structures*, 2nd ed., Interscience, New York, 1963. In most cases, the data are taken at about room temperature and normal atmospheric pressure. For elements that exist in many forms the stable room temperature form (or forms) is given. For more detailed information, more precise lattice constants, and references, the Wyckoff work should be consulted.

body centered cubic (bcc)

Table 4.2
ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

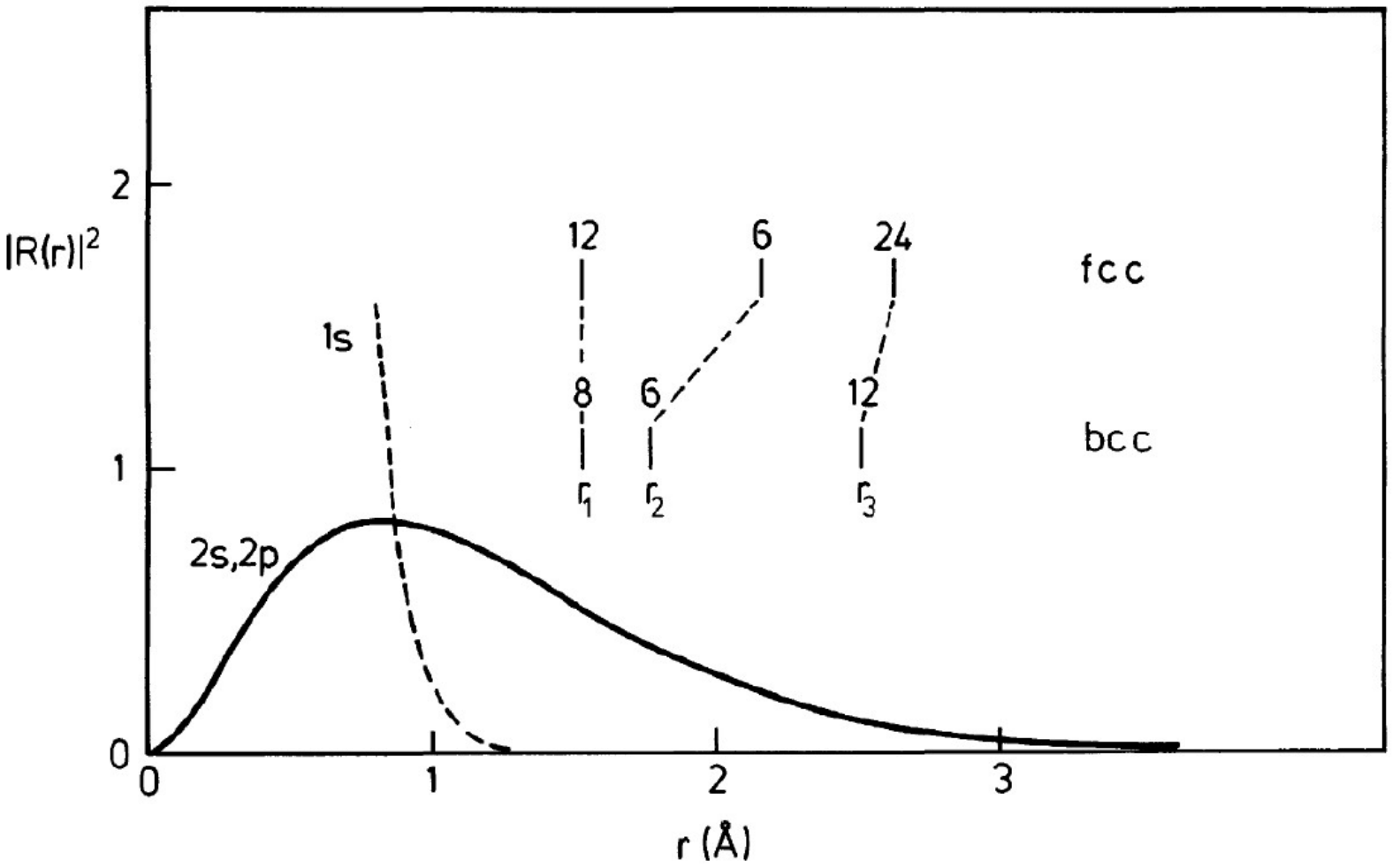
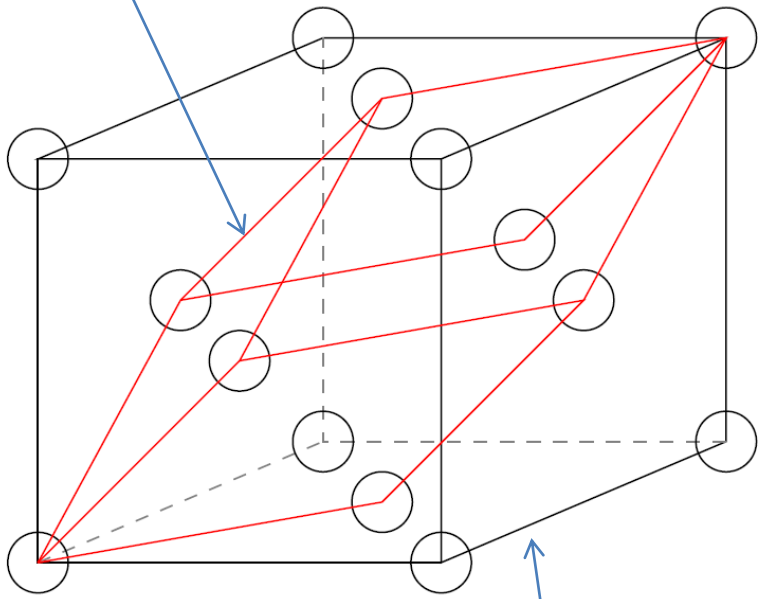


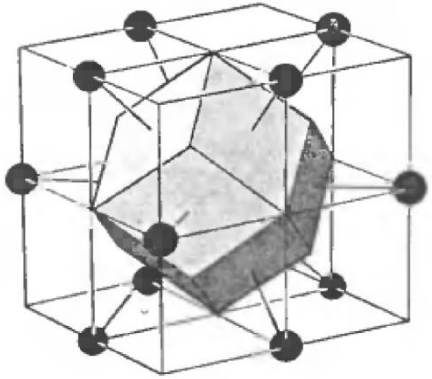
Figure 2.13: Lithium wave functions versus distance

face centered cubic

primitive unit cell

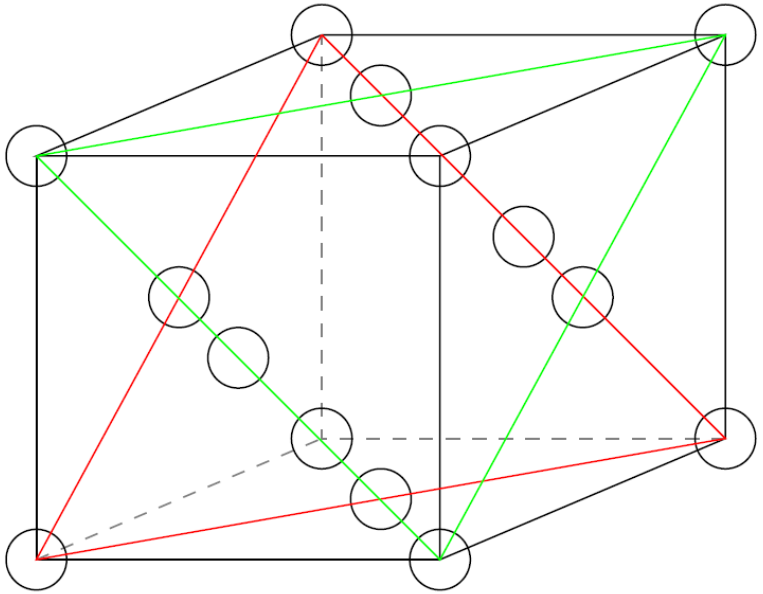


conventional unit cell



Wigner Seitz Cell

Lattice Planes & Miller Indices



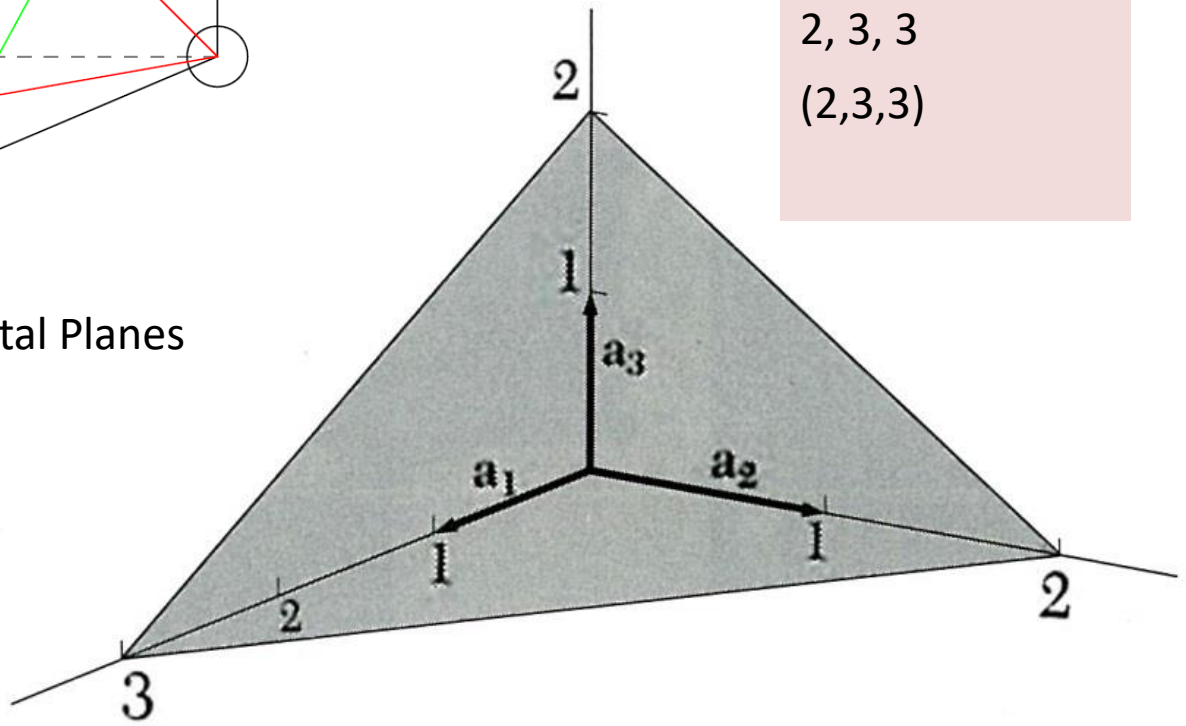
$3a_1$, $2a_2$, $2a_3$

1/3, 1/2, 1/2

2, 3, 3

(2,3,3)

Crystal Planes



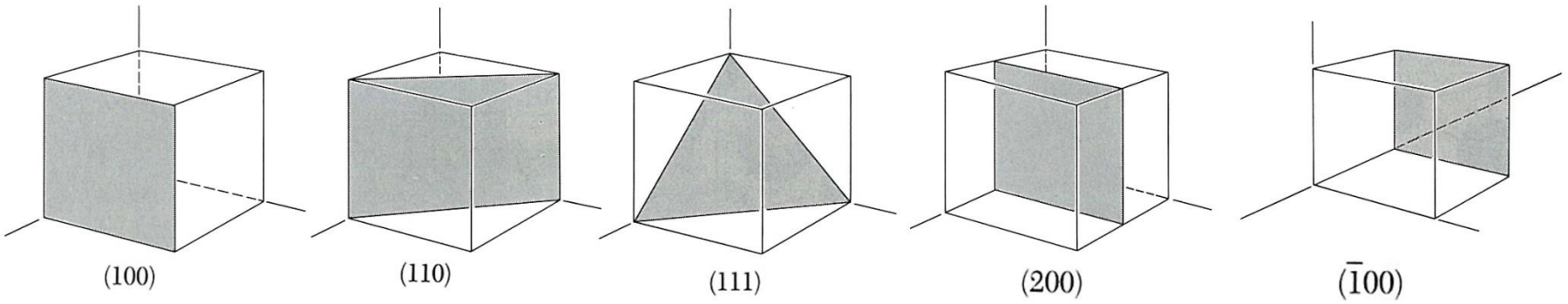


Figure 16 Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to (1̄00).

(h k l) – denotes a plane (or a set of planes)

[h k l] – denotes a direction

For cubic systems: [h k l] perpendicular to (h k l)

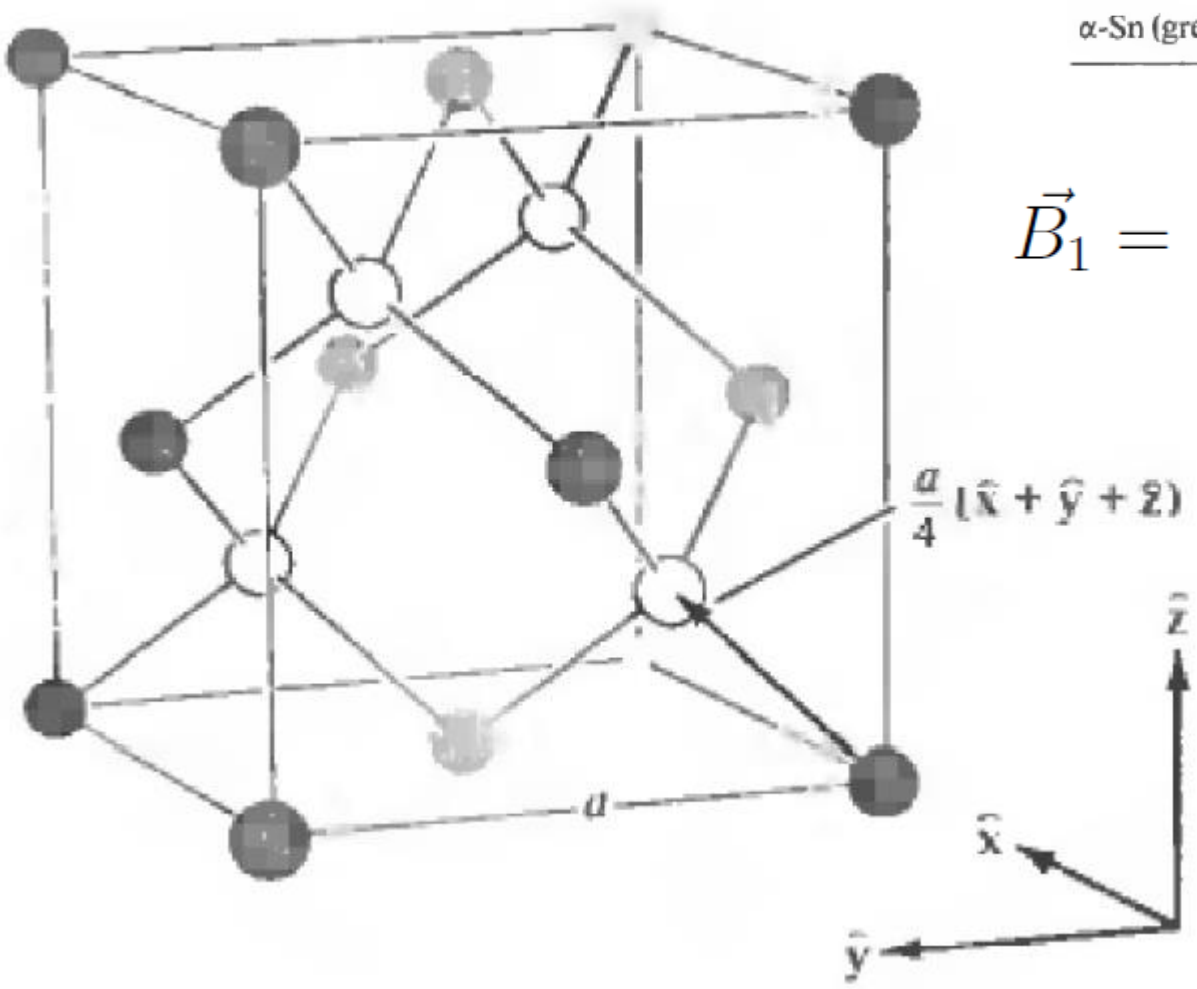
Simple Crystal Structures

Diamond Structure
(typical for covalent sp^3 systems – tetrahedral bond)

ELEMENTS WITH THE DIAMOND CRYSTAL STRUCTURE

ELEMENT	CUBE SIDE a (Å)
C (diamond)	3.57
Si	5.43
Ge	5.66
α-Sn (grey)	6.49

$$\vec{B}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} ; \vec{B}_2 = \begin{pmatrix} a/4 \\ a/4 \\ a/4 \end{pmatrix}$$



Filling Factor = 0.34, 4 nearest neighbors

hexagonal close-packed structure (hcp)

$$\vec{B}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} ; \vec{B}_2 = \begin{pmatrix} a/3 \\ a/3 \\ a/2 \end{pmatrix}$$

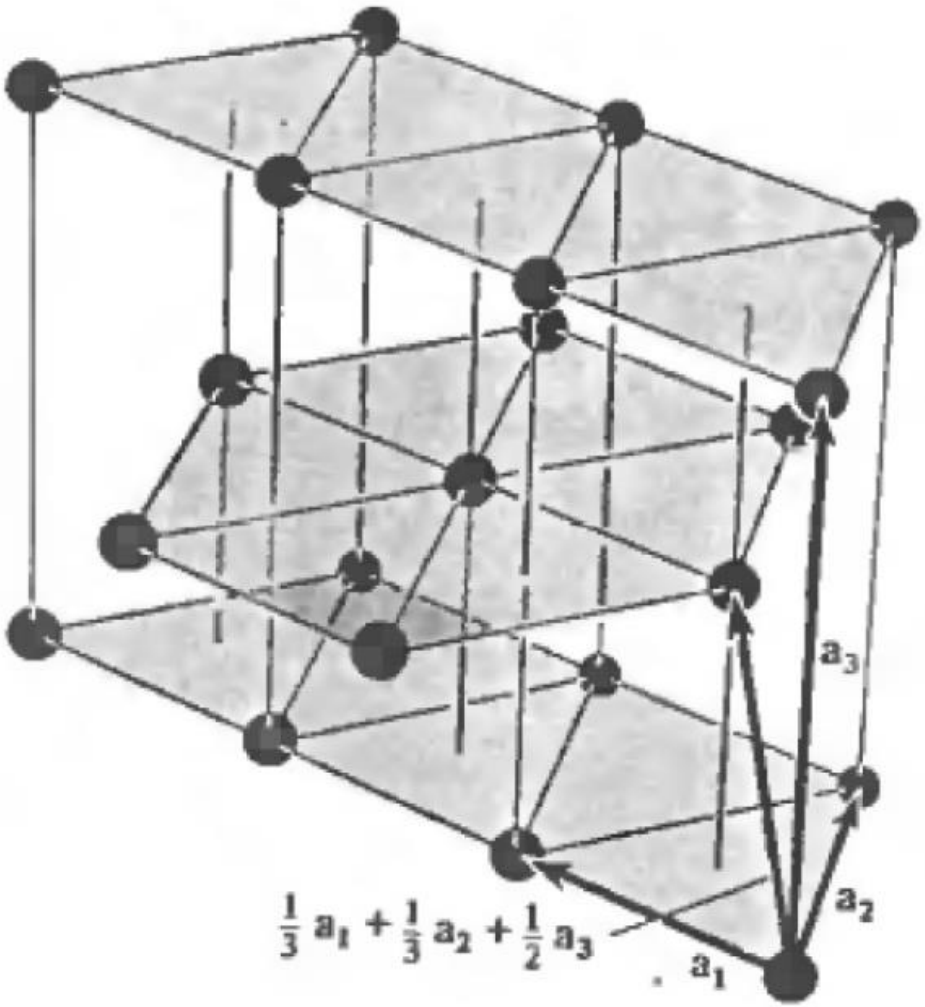
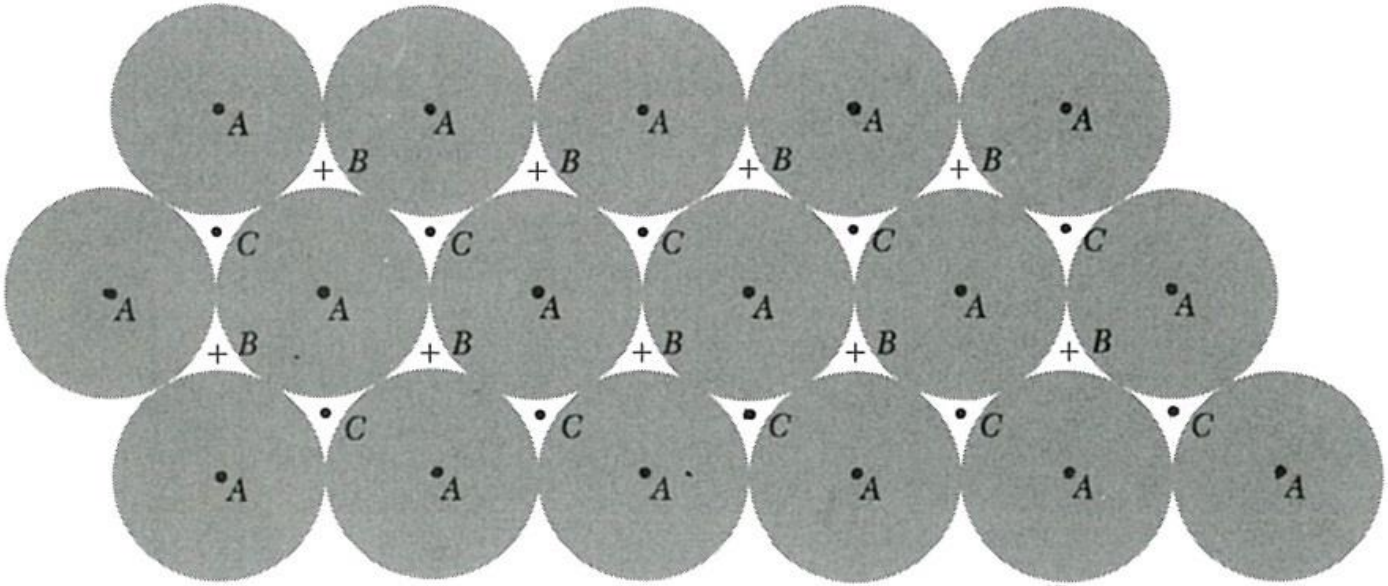


Table 4.4
ELEMENTS WITH THE HEXAGONAL CLOSE-PACKED CRYSTAL STRUCTURE

ELEMENT	a (Å)	c	c/a	ELEMENT	a (Å)	c	c/a
Be	2.29	3.58	1.56	Os	2.74	4.32	1.58
Cd	2.98	5.62	1.89	Pr	3.67	5.92	1.61
Ce	3.65	5.96	1.63	Re	2.76	4.46	1.62
α-Co	2.51	4.07	1.62	Ru	2.70	4.28	1.59
Dy	3.59	5.65	1.57	Sc	3.31	5.27	1.59
Er	3.56	5.59	1.57	Tb	3.60	5.69	1.58
Gd	3.64	5.78	1.59	Ti	2.95	4.69	1.59
He (2 K)	3.57	5.83	1.63	Tl	3.46	5.53	1.60
Hf	3.20	5.06	1.58	Tm	3.54	5.55	1.57
Ho	3.58	5.62	1.57	Y	3.65	5.73	1.57
La	3.75	6.07	1.62	Zn	2.66	4.95	1.86
Lu	3.50	5.55	1.59	Zr	3.23	5.15	1.59
Mg	3.21	5.21	1.62		—	—	
Nd	3.66	5.90	1.61	"Ideal"			1.63



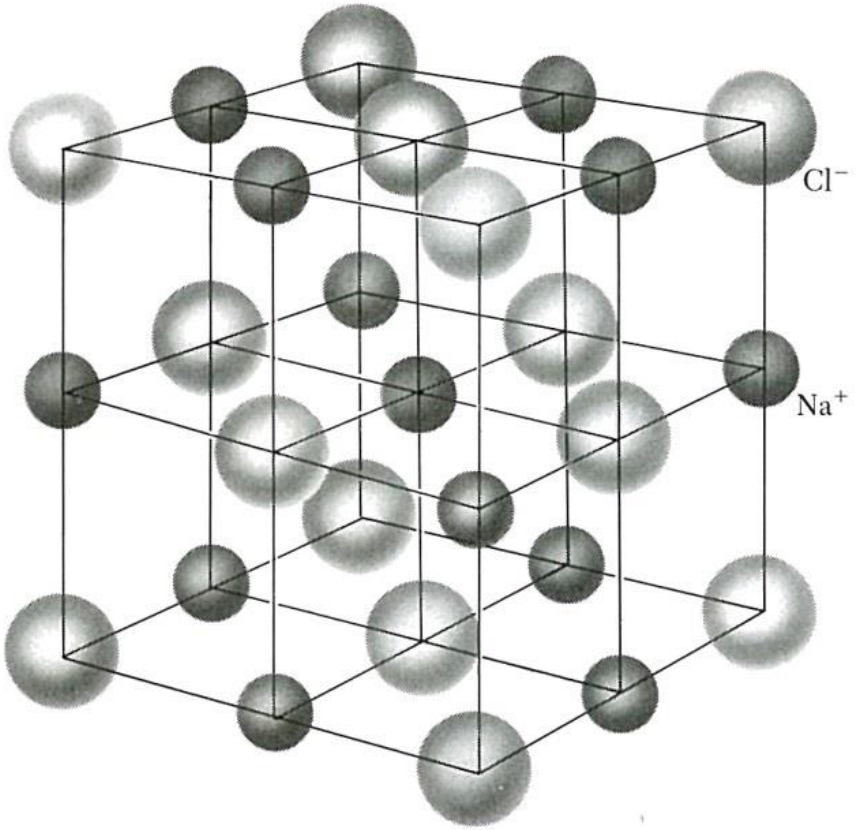
hcp: **ABABAB**

fcc: **ABCABC**

Figure 21 A close-packed layer of spheres is shown, with centers at points marked *A*. A second and identical layer of spheres can be placed on top of this, above and parallel to the plane of the drawing, with centers over the points marked *B*. There are two choices for a third layer. It can go in over *A* or over *C*. If it goes in over *A* the sequence is *ABABAB*. . . and the structure is hexagonal close-packed. If the third layer goes in over *C* the sequence is *ABCABCABC*. . . and the structure is face-centered cubic.

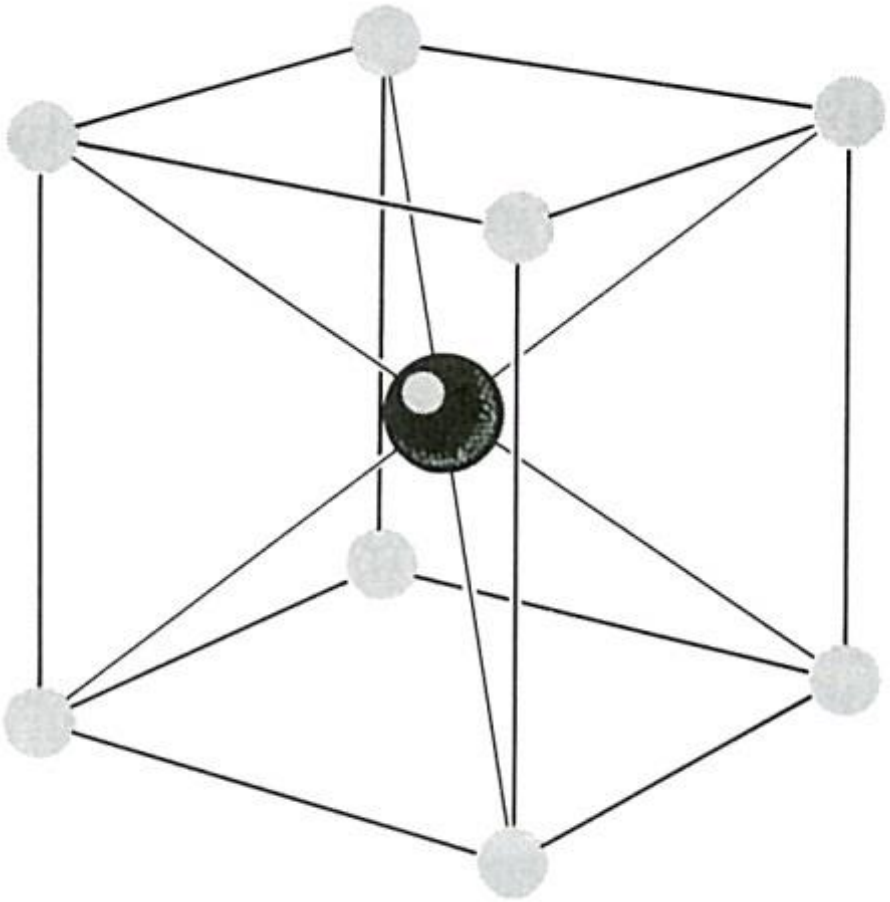
Sodium Chloride Structure: fcc with 2 atomic basis (1 x Cl- & 1 x Na+)

Cl:	000 ;	$\frac{1}{2}\frac{1}{2}0$;	$\frac{1}{2}0\frac{1}{2}$;	$0\frac{1}{2}\frac{1}{2}$.
Na:	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$;	$00\frac{1}{2}$;	$0\frac{1}{2}0$;	$\frac{1}{2}00$.



each atom has 6 neighbors

Cesium Chloride Structure



Cs+ at 000

Cl- at ½, ½, ½

8 neighbours

Zincblende Structure (diamond with 2 atomic base) or zinc sulfide structure

Table 4.7
SOME COMPOUNDS WITH THE ZINCBLENDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
CuF	4.26	ZnS	5.41	AlSb	6.13
CuCl	5.41	ZnSe	5.67	GaP	5.45
CuBr	5.69	ZnTe	6.09	GaAs	5.65
CuI	6.04	CdS	5.82	GaSb	6.12
AgI	6.47	CdTe	6.48	InP	5.87
BeS	4.85	HgS	5.85	InAs	6.04
BeSe	5.07	HgSe	6.08	InSb	6.48
BeTe	5.54	HgTe	6.43	SiC	4.35
MnS (red)	5.60	AlP	5.45		
MnSe	5.82	AlAs	5.62		

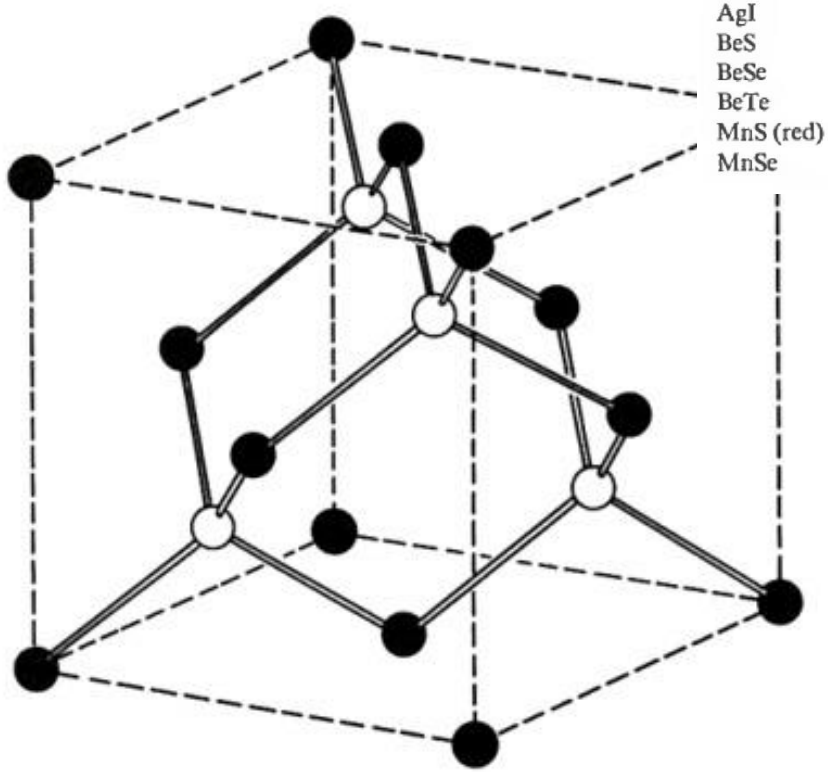
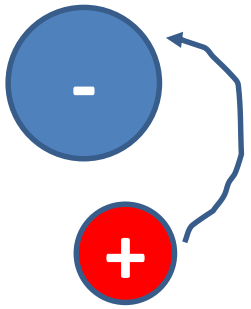


Figure 26 Crystal structure of cubic zinc sulfide.

Ionic crystals:

Sodium Chloride Structure
Cesium Chloride Structure
Zincblende Structure

?!



charge transfer

Potential Energy

$$V_i = \frac{e}{4\pi\epsilon_0} \sum_{j \neq i} \frac{z_j}{r_{ij}}$$

z_j = number of charges of the jth ion
e = 1.6x10-19 C
r_{ij} = distance between ith and jth ion

Madelung Constant

$$M_i = \sum_j \frac{z_j}{r_{ij}/r_0}.$$

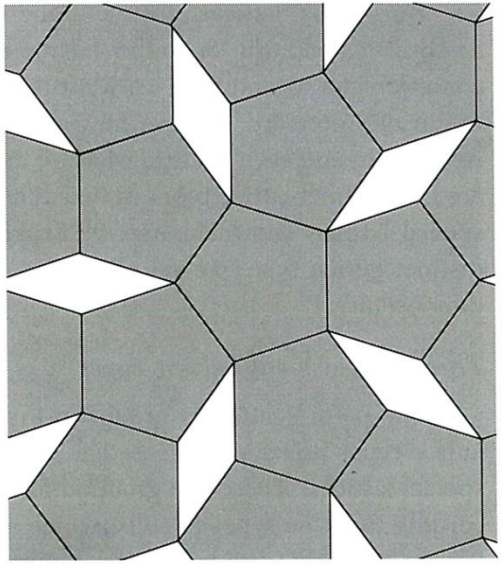
M < 1.634 Zincblende
M > 1.763 CsCl
1.634 < M < 1.763 NaCl

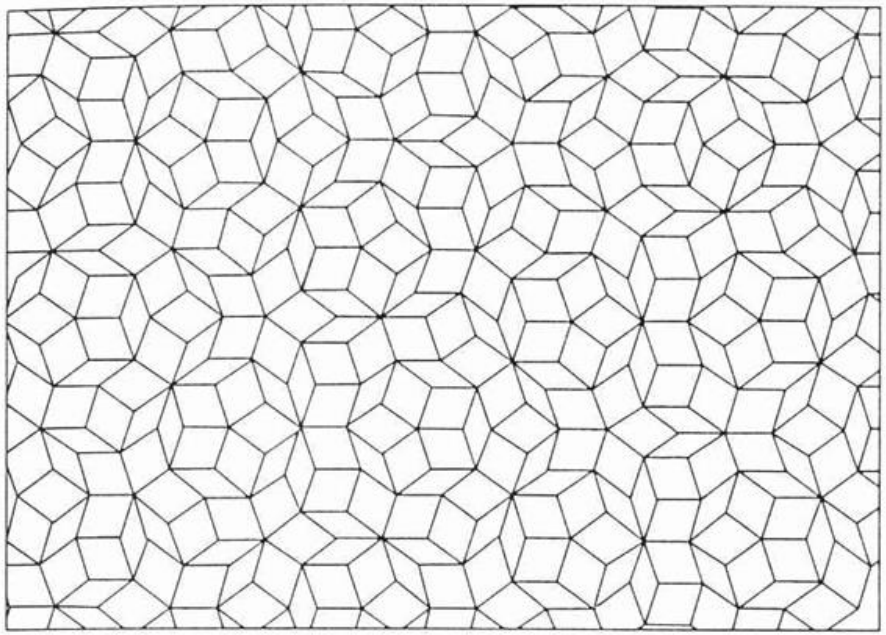
Lattices can only have 1-,2-,4-,6- fold rotational symmetry

Five fold symmetry ?

Quasi-crystal !

Figure 7 A fivefold axis of symmetry cannot exist in a periodic lattice because it is not possible to fill the area of a plane with a connected array of pentagons. We can, however, fill all the area of a plane with just two distinct designs of "tiles" or elementary polygons. A quasicrystal is a quasiperiodic nonrandom assembly of two types of figures. Quasicrystals are discussed at the end of Chapter 2.





Penrose tiling

Figure 19 A quasicrystal tiling in two dimensions, after the work of Penrose. The long-range orientational order and the long-range non-periodic order are shown.