Chapter 2 Crystal Structures
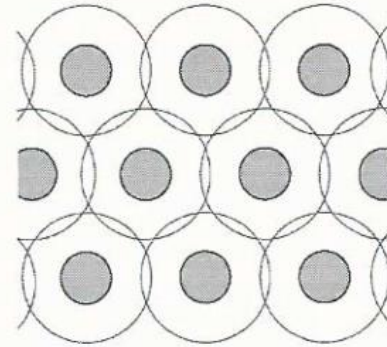
2.1 Introduction

1. Solids and their types

a) What is a solid:
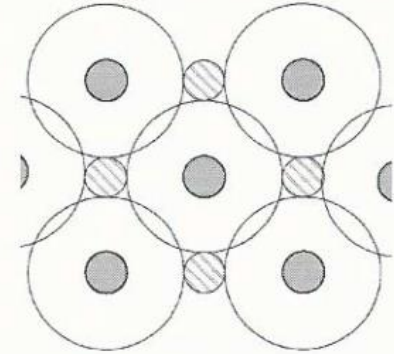
A solid = atoms + chemical bond(s)
(collection) (atomic glue(s))
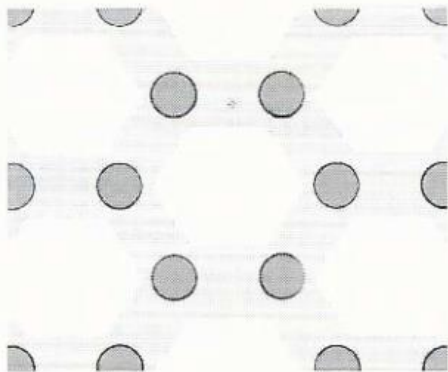

Van der Waals-like
(rare gas solids)

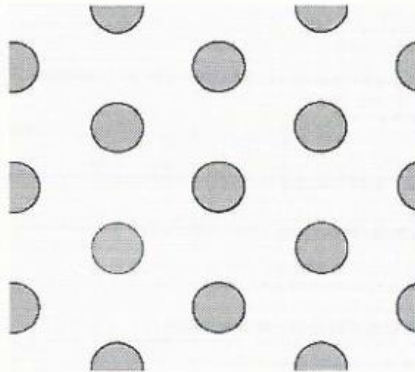Ionic bonding
(NaCl)
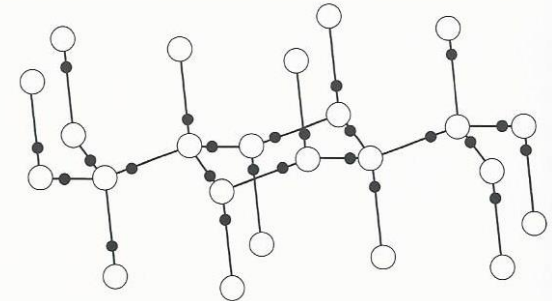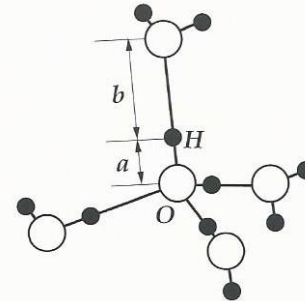
Covalent bonding
(diamond, silicon)

Metallic bonding
(Na, Cu)

(e) hydrogen bonding (ice)

b) Types of materials
(1) crystalline solids:
   atoms (molecules or atomic clusters) sitting on a regular lattice (long range order).

MgB$_2$

simple hcp
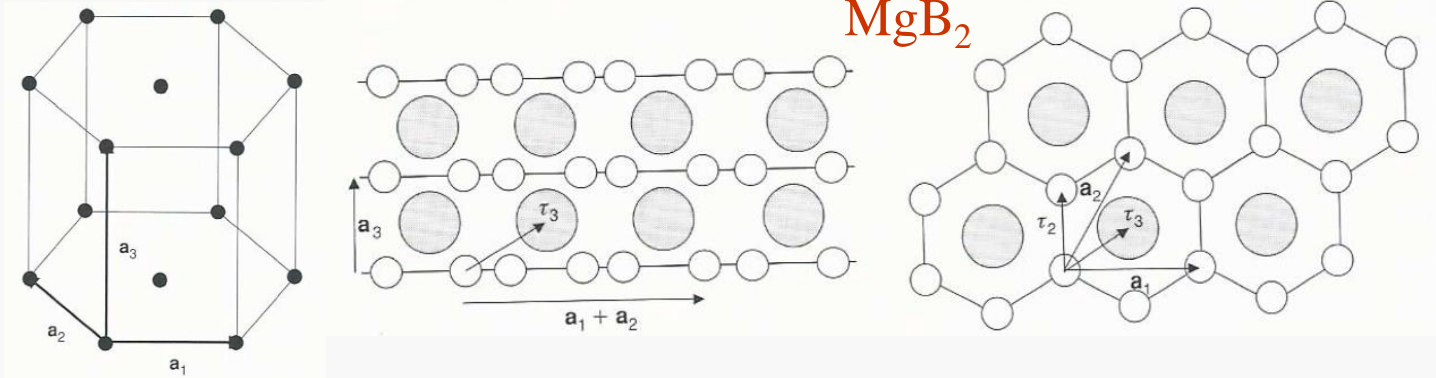
(2) Amorphous materials:
   non-crystalline solids (short range order, e.g., regular local coordination), e.g., glasses (e.g., SiO$_2$)

Si
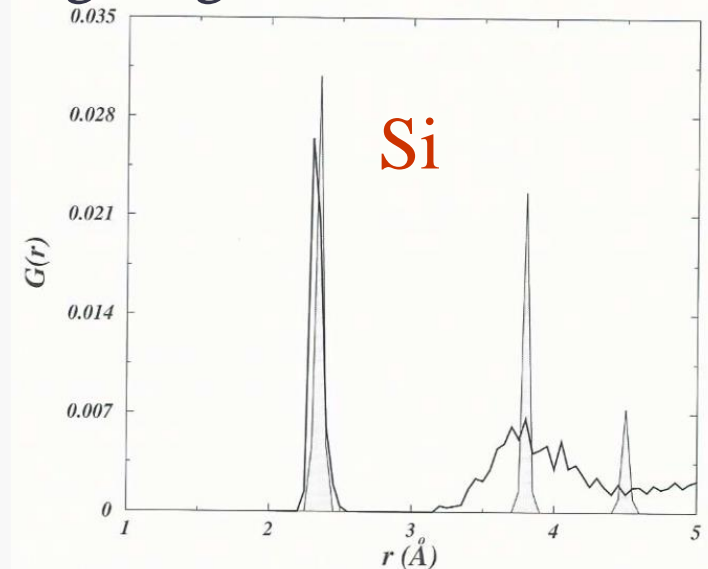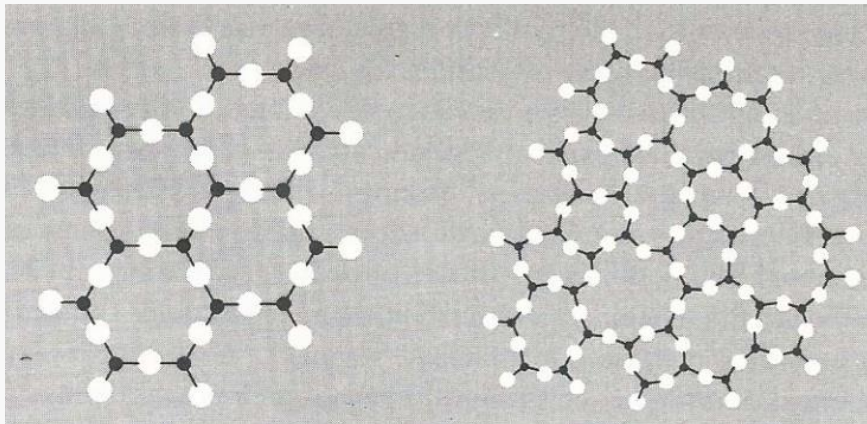
Radial distribution $4\pi r^2 \rho(r)$ for liquid (curve) and crystalline (vertical lines) sodium.

(3) Quasi-crystals:
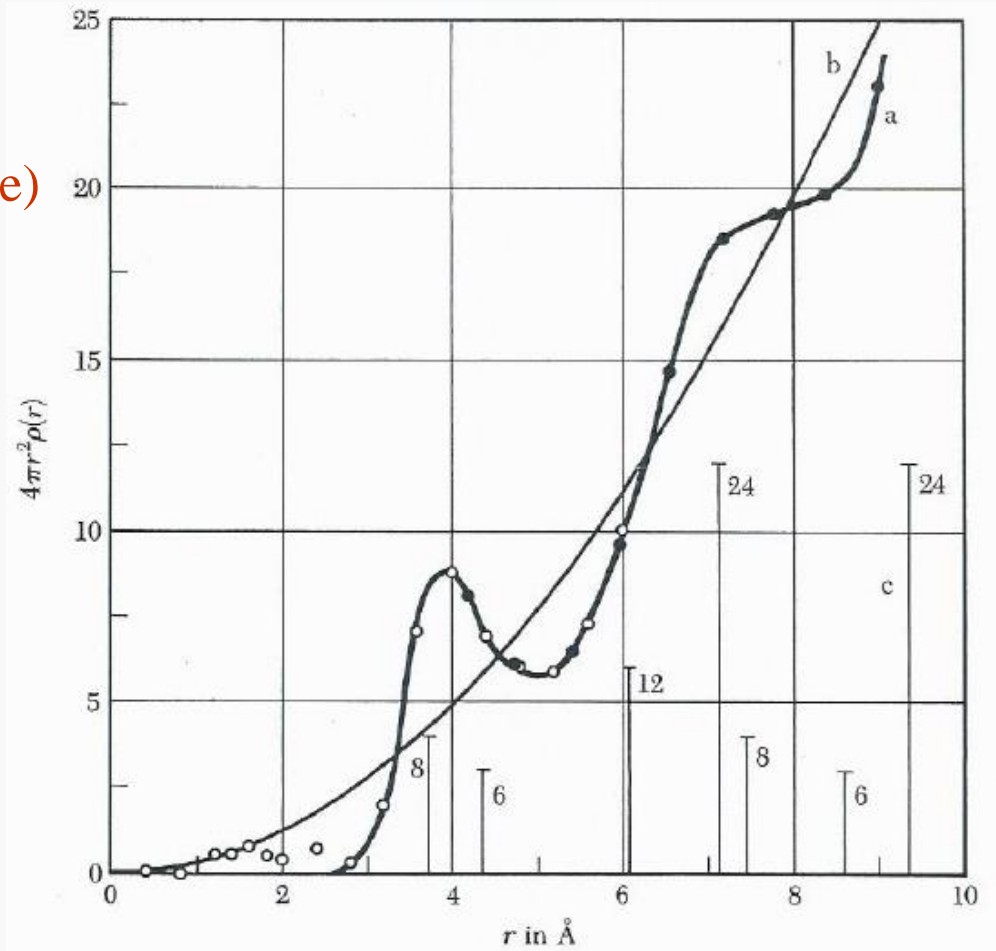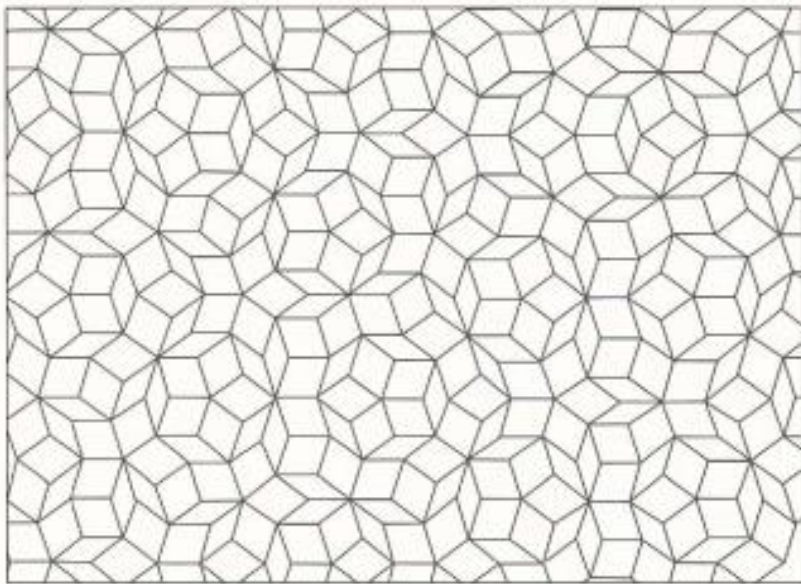
Penrose tile (2D-quasicrystal)

Real materials:
A crystal + imperfections (e.g., lattice vibrations, point defects, impurities, surface/interface, finite sizes, etc).

2. Solid state and materials physics

a) **Investigation of mainly collective properties of the atoms in a solid**

MATERIAL	T_c (K)	M_0 (gauss)[a]
Fe	1043	1752
Co	1388	1446
Ni	627	510
Gd	293	1980
Dy	85	3000
$CrBr_3$	37	270
Au_2MnAl	200	323
Cu_2MnAl	630	726
Cu_2MnIn	500	613
EuO	77	1910
EuS	16.5	1184
MnAs	318	870
MnBi	670	675
$GdCl_3$	2.2	550

[a] At $T = 0(K)$.
Source: F. Keffer, *Handbuch der Physik*, vol. 18, pt. 2, Springer, New York, 1966; P. Heller, *Rep. Progr. Phys.*, **30**, (pt. II), 731 (1967).

[a] Elements that are superconducting only under special conditions are indicated separately. Note the incompatibility of superconducting and magnetic order. After G. Gladstone, et al. Parks *op. cit*, note 6.

Legend:

Al	Superconducting
B	Nonmetallic elements
Si	Superconducting under high pressure or in thin films
Fe	Elements with magnetic order
Li	Metallic but not yet found to be superconducting

b) Physical properties of solids

(1) characteristic properties of the constituent atoms influenced by the surroundings (intrinsic atomic properties).
(2) new properties (i.e., not due to an individual atom):
    e.g., structural and mechanical properties, magnetism, electrical property (conductor, semiconductor, insulator, superconductor).

c) Typical questions

(1) What is the ground state (structure) of a given solid?
    (low T and ambient pressure)
    Why is it stable?
    What sort of forces (chemical bonds) hold the atoms together in the
     lattice?
(2) How does a solid behave under external influences?
    electrical field => conductivity
    temperature gradient => thermal conductivity
    pressure => bulk moduli, structural phase transition etc
    magnetic field => magnetic susceptibility
    light field => optical properties
    etc.

3. Characteristics of theoretical methods

Two principal properties of solid materials

(1) Translational (& point group) symmetry of the crystalline lattice:
This allows one to consider only a few atoms in a primitive cell by introducing band theory.

(2) A many-body system of nuclei and electrons (not few-body problems):
This allows one to use powerful statistical mechanics methods (e.g., Fermi-Dirac statistics) and also effective mean-field theories (e.g., density functional theory).

2.2 Crystals and their symmetries

1. Description (definition) of a crystal
   An ideal crystal is constructed by the infinite repetition of identical structure units (unit cells) in space.

(a)   (b)
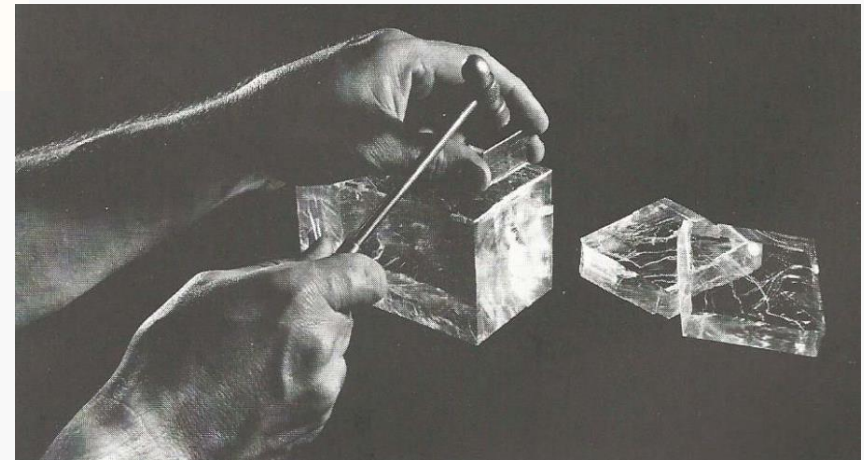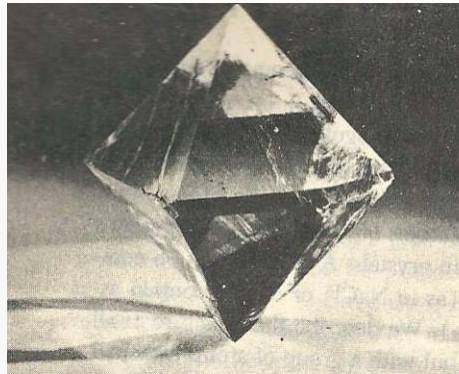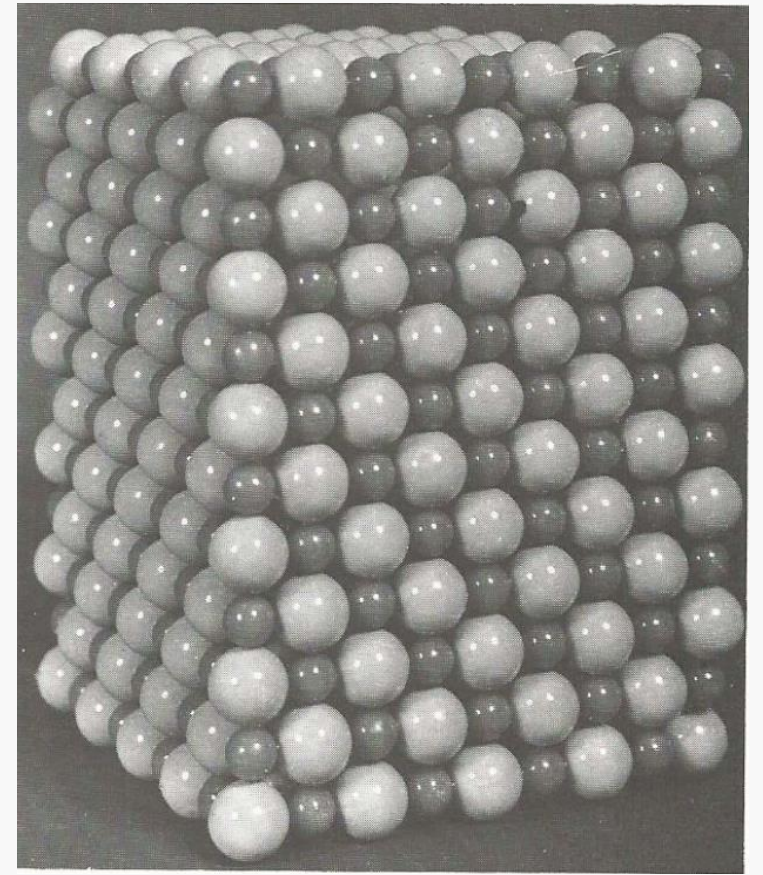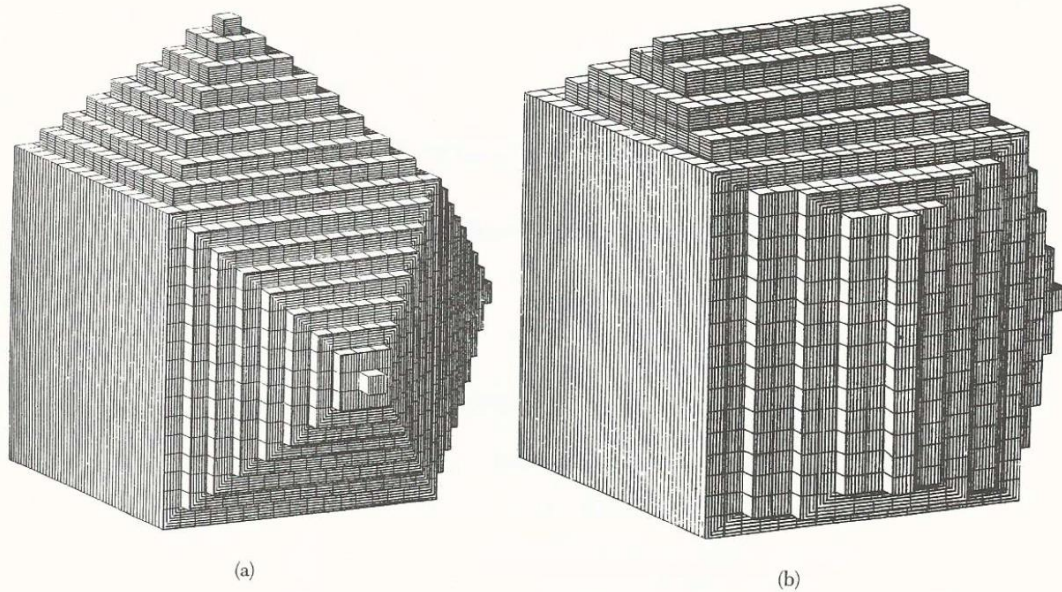
A crystal structure = a lattice + a basis.
A lattice consists of all points with
position vectors

$$\mathbf{R}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3,$$

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$: primitive vectors,

n_1, n_2, n_3 : integers.

$\mathbf{a}_2$

unit cell
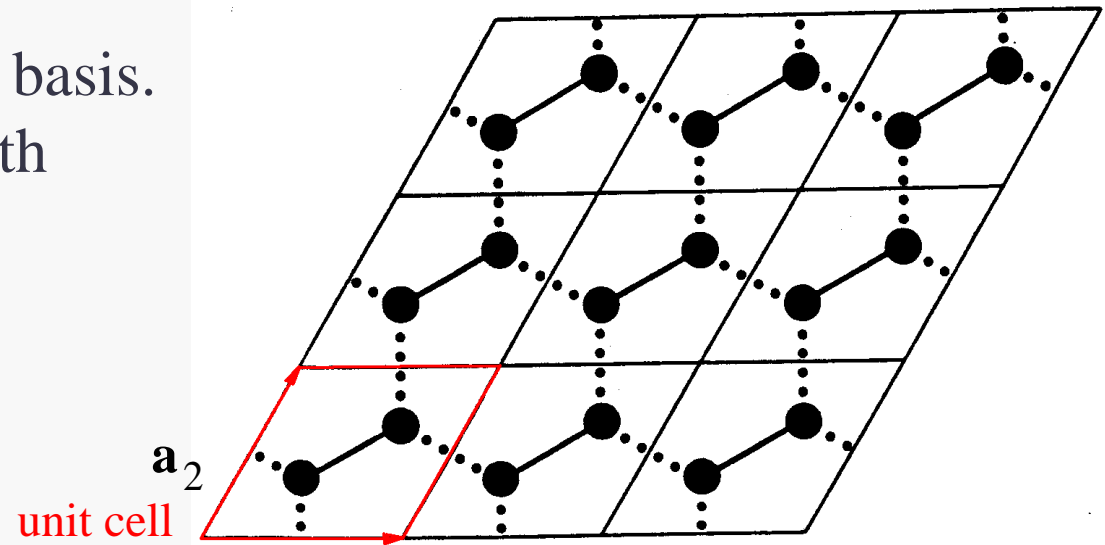
$\mathbf{a}_1$ A 2D hexagonal crystal (graphene)

A basis consists of either a single atom, a
molecule or a cluster of atoms and is
attached to every lattice point. The atomic
positions in the basis are given:

$$\boldsymbol{\tau}_i = x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_3 \mathbf{a}_3,$$

where $0 \leq x_1, x_2, x_3 \leq 1$.
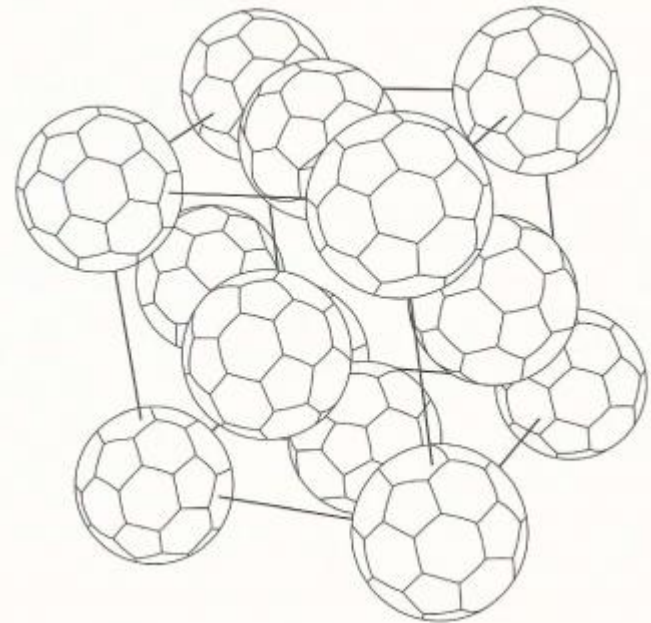
fcc crystal structure of C_{60} molecules

Wigner-Seitz cell:
There are many ways to specify a unit cell.

A standard way to construct is as follows.
Starting from one lattice point as the origin, draw connecting lines to all other $\mathbf{R}_m$s, the planes erected at the mid-points of these lines define the boundaries of the unit cell.
The resultant unit cell is called the Wigner-Seitz cell. The Wigner-Seitz cell has the symmetry of the crystal structure (i.e., invariant to all lattice symmetry operations, rotations, reflections, inversions).
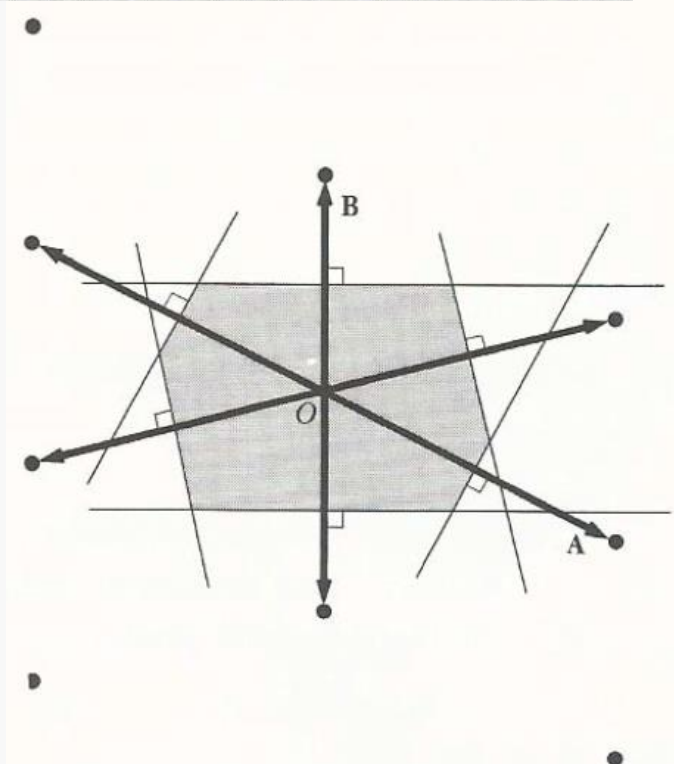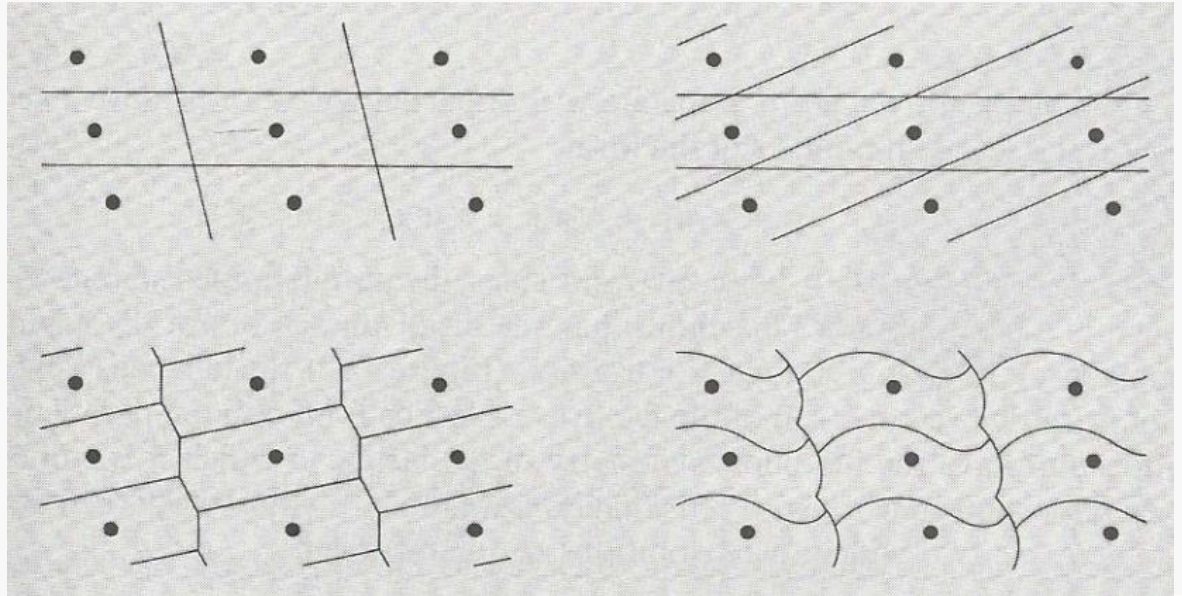
Examples of crystal lattices
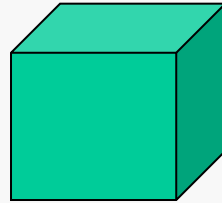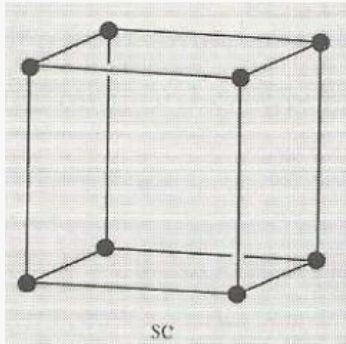
cesium chloride structure
CsCl, AgMg, AlNi, CuPd

a. Simple cubic lattice (sc)

$$\mathbf{a}_1 = a\hat{i}$$

$$\mathbf{a}_2 = a\hat{j}$$

$$\mathbf{a}_3 = a\hat{k}$$

Wigner-Seitz cell

Perovskite ABO_3 structure
$BaTiO_3$, $SrTiO_3$, $CaMnO_3$
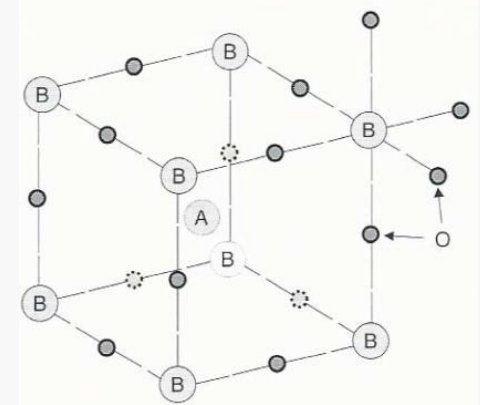
b. Body center cubic lattice (bcc)

$$\mathbf{a}_1 = \frac{a}{2}\left(-\vec{i} + \vec{j} + \vec{k}\right)$$
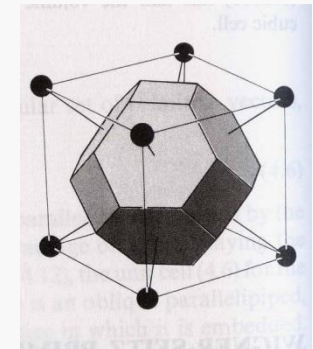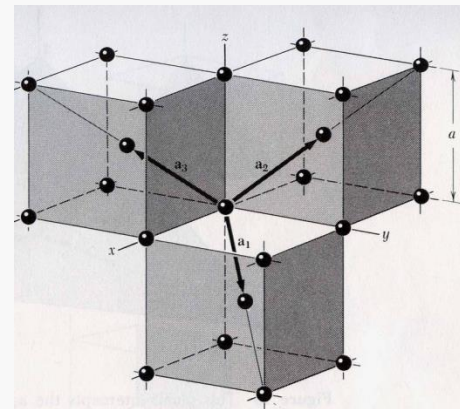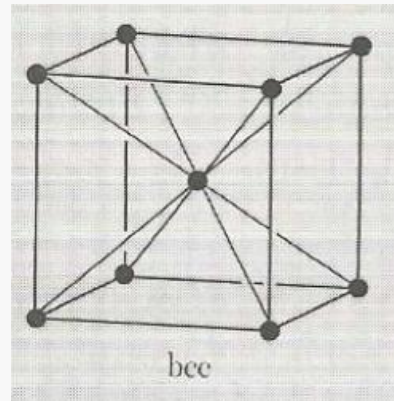
$$\mathbf{a}_2 = \frac{a}{2}\left(\vec{i} - \vec{j} + \vec{k}\right)$$

$$\mathbf{a}_3 = \frac{a}{2}\left(\vec{i} + \vec{j} - \vec{k}\right)$$

Wigner-Seitz cell

e.g., chromium (Cr), iron (Fe)

c. Face centered cubic lattice (fcc)

$$\mathbf{a}_1 = \frac{a}{2}\left(\vec{j} + \vec{k}\right)$$

$$\mathbf{a}_2 = \frac{a}{2}\left(\vec{i} + \vec{k}\right)$$

$$\mathbf{a}_3 = \frac{a}{2}\left(\vec{i} + \vec{j}\right)$$
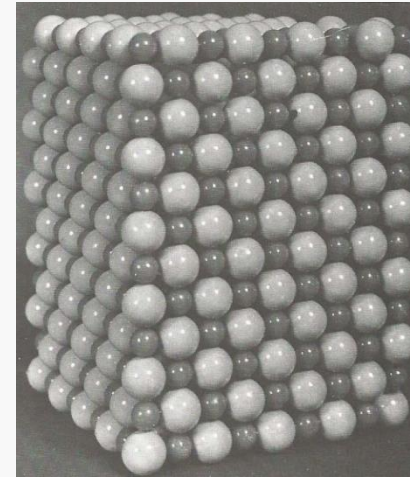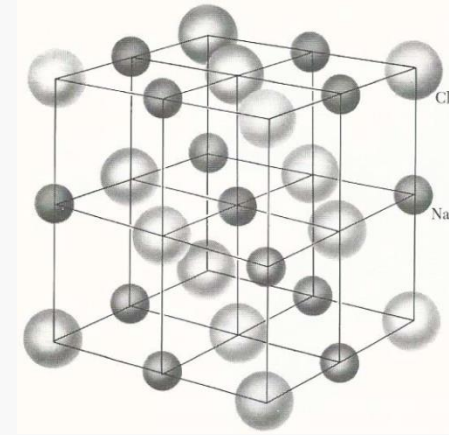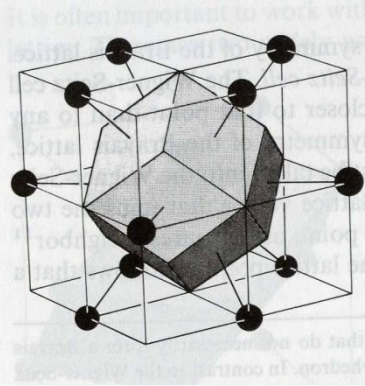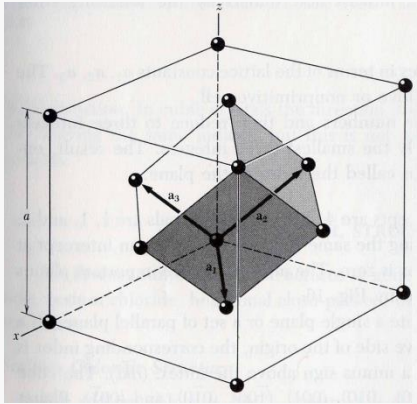
e.g., Sodium chloride structure
NaCl, LiH, MnO, KCl, KBr

e.g., Diamond structure
Diamond, Si, Ge
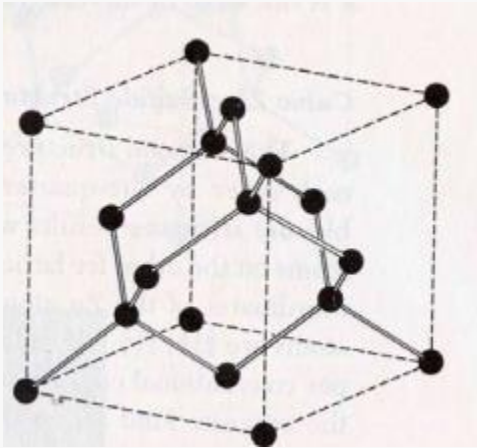
e.g., Zincblende structure
ZnS, GaAs, SiC, ZnS
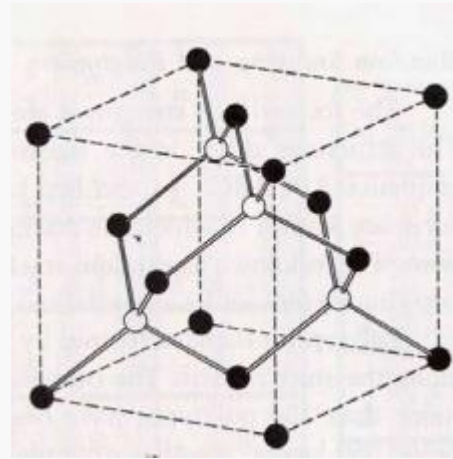
d. Hexagonal lattice (hcp)

e.g., Co, Zn, Cd

$$\vec{a}_1 = a\left(\frac{1}{2}\vec{i} + \frac{\sqrt{3}}{2}\vec{j}\right)$$

$$\vec{a}_2 = a\left(\frac{1}{2}\vec{i} - \frac{\sqrt{3}}{2}\vec{j}\right)$$

$$\vec{a}_3 = c\vec{k}$$

c/a = 1.633

2H-MoS$_2$ (C7)

2H-NbS$_2$

GROUP P6$_3$/mmc - D$_{6h}^4$

P6$_3$/m mc - D$_{6h}^4$
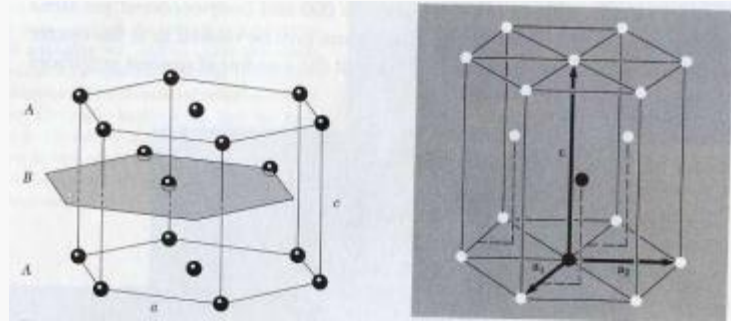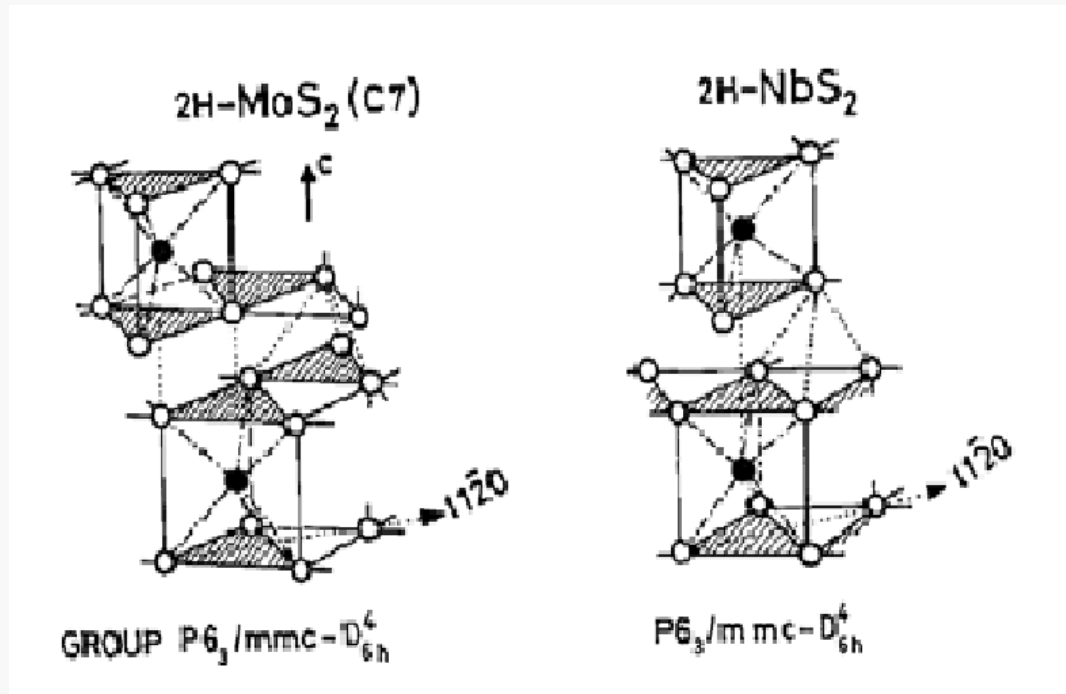
Table 3 Crystal structures of the elements

The data given are at room temperature for the most common form, or at the stated temperature in deg K. For further descriptions of the elements see Wyckoff, Vol. 1, Chap. 2. Structures labeled complex are described there.

Legend: Crystal structure / a lattice parameter, in Å / c lattice parameter, in Å

Element	Structure	a	c
H¹ (4K)	hcp	3.75	6.12
He⁴ (2K)	hcp	3.57	5.83
Li (78K)	bcc	3.491	
Be	hcp	2.27	3.59
B	rhomb.		
C	diamond	3.567	
N (20K)	cubic	5.66 (N_2)	
O	complex (O_2)		
F			
Ne (4K)	fcc	4.46	
Na (5K)	bcc	4.225	
Mg	hcp	3.21	5.21
Al	fcc	4.05	
Si	diamond	5.430	
P	complex		
S	complex		
Cl	complex (Cl_2)		
Ar (4K)	fcc	5.31	
K (5K)	bcc	5.225	
Ca	fcc	5.58	
Sc	hcp	3.31	5.27
Ti	hcp	2.95	4.68
V	bcc	3.03	
Cr	bcc	2.88	
Mn	cubic complex		
Fe	bcc	2.87	
Co	hcp	2.51	4.07
Ni	fcc	3.52	
Cu	fcc	3.61	
Zn	hcp	2.66	4.95
Ga	complex		
Ge	diamond	5.658	
As	rhomb.		
Se	hex. chains		
Br	complex (Br_2)		
Kr (4K)	fcc	5.64	
Rb (5K)	bcc	5.585	
Sr	fcc	6.08	
Y	hcp	3.65	5.73
Zr	hcp	3.23	5.15
Nb	bcc	3.30	
Mo	bcc	3.15	
Tc	hcp	2.74	4.40
Ru	hcp	2.71	4.28
Rh	fcc	3.80	
Pd	fcc	3.89	
Ag	fcc	4.09	
Cd	hcp	2.98	5.62
In	tetr.	3.25	4.95
Sn (α)	diamond	6.49	
Sb	rhomb.		
Te	hex. chains		
I	complex (I_2)		
Xe (4K)	fcc	6.13	
Cs (5K)	bcc	6.045	
Ba	bcc	5.02	
La	hex.	3.77	ABAC
Hf	hcp	3.19	5.05
Ta	bcc	3.30	
W	bcc	3.16	
Re	hcp	2.76	4.46
Os	hcp	2.74	4.32
Ir	fcc	3.84	
Pt	fcc	3.92	
Au	fcc	4.08	
Hg	rhomb.		
Tl	hcp	3.46	5.52
Pb	fcc	4.95	
Bi	rhomb.		
Po	sc	3.34	
At	—		
Rn	—		
Fr	—		
Ra	—		
Ac	fcc	5.31	

Lanthanides:

Element	Structure	a	c
Ce	fcc	5.16	
Pr	hex.	3.67	ABAC
Nd	hex.	3.66	
Pm	—		
Sm	complex		
Eu	bcc	4.58	
Gd	hcp	3.63	5.78
Tb	hcp	3.60	5.70
Dy	hcp	3.59	5.65
Ho	hcp	3.58	5.62
Er	hcp	3.56	5.59
Tm	hcp	3.54	5.56
Yb	fcc	5.48	
Lu	hcp	3.50	5.55

Actinides:

Element	Structure	a	c
Th	fcc	5.08	
Pa	tetr.	3.92	3.24
U	complex		
Np	complex		
Pu	complex		
Am	hex.	3.64	ABAC
Cm	—		
Bk	—		
Cf	—		
Es	—		
Fm	—		
Md	—		
No	—		
Lr	—		

2. Translational symmetry

The periodicities of a crystal structure means that the crystal is invariant to any translation $\mathbf{R}$ over distances which are multiples of the basis vectors ($\mathbf{R} \in \{\mathbf{R}_n\}$). All these translations constitute an Abelian group called the translational group ($\{E|\mathbf{R}_n\}$).

This symmetry implies that all the ground state properties of the crystal are invariant under the translational operations.
For example, $\rho(\mathbf{r} + \mathbf{R}_n) = \rho(\mathbf{r})$.

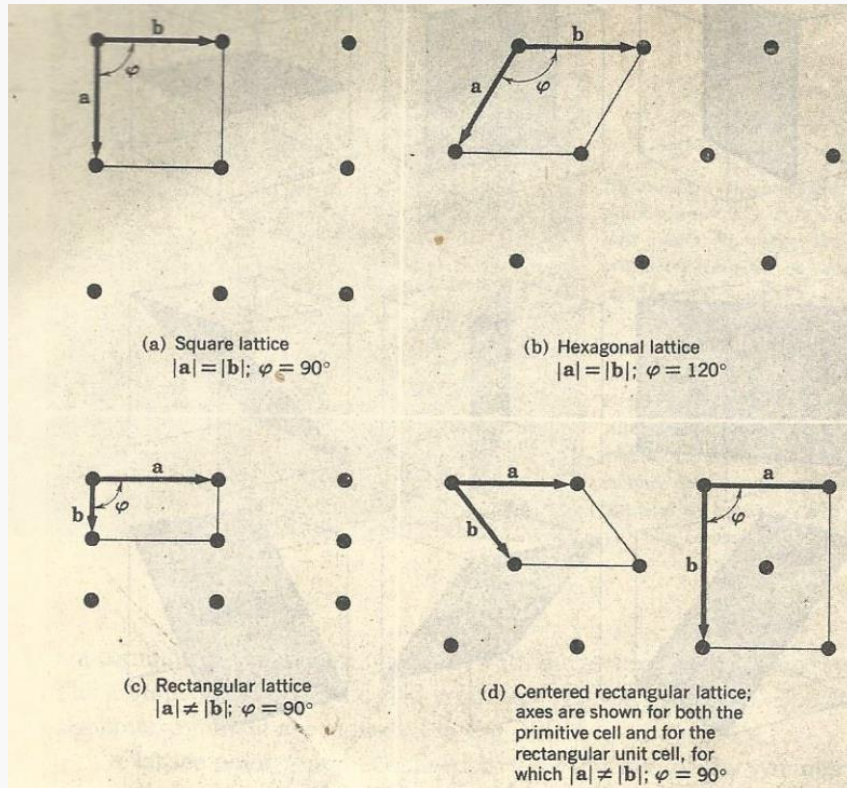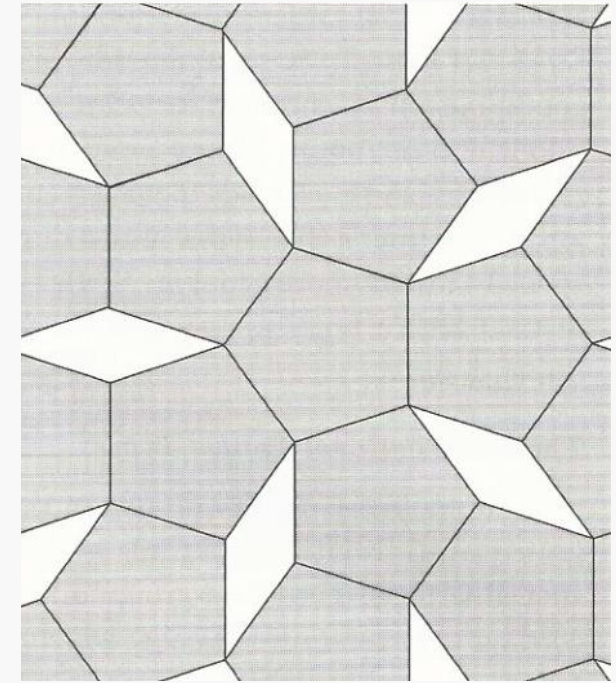This translational symmetry is fundamentally important for general theories of solids.

3. Point (group) symmetries

In addition to the translational symmetry, some point-group operations such as rotations and reflection also leave a crystal unchanged. Not all point-group operations would leave the crystal invariant.

(a) Square lattice
$|a| = |b|$; $\varphi = 90°$

(b) Hexagonal lattice
$|a| = |b|$; $\varphi = 120°$

(c) Rectangular lattice
$|a| \neq |b|$; $\varphi = 90°$

(d) Centered rectangular lattice; axes are shown for both the primitive cell and for the rectangular unit cell, for which $|a| \neq |b|$; $\varphi = 90°$

A fivefold rotation axis cannot exist in a lattice.

There are five groups for 2D point lattices and ten groups for 2D crystal structures.

Lattice	Conventional cell	Axes of coventional cell	Point-group symmetry of lattice about lattice points
Oblique	Parallelogram	$a \neq b$, $\varphi \neq 90°$	2
Square	Square	$a = b$, $\varphi = 90°$	4mm
Hexagonal	60° rhombus	$a = b$, $\varphi = 120°$	6mm
Primitive rectangular	Rectangle	$a \neq b$, $\varphi = 90°$	2mm
Centered rectangular	Rectangle	$a \neq b$, $\varphi = 90°$	2mm

There are 32 point groups for 3D crystal structures.
There are 7 crystal systems and
14 Bravais lattices.

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	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$

Cubic P   Cubic I   Cubic F
Tetragonal P   Tetragonal I
Orthorhombic P   Orthorhombic C   Orthorhombic I   Orthorhombic F
Monoclinic P   Monoclinic C   Triclinic
Trigonal R   Trigonal and Hexagonal P
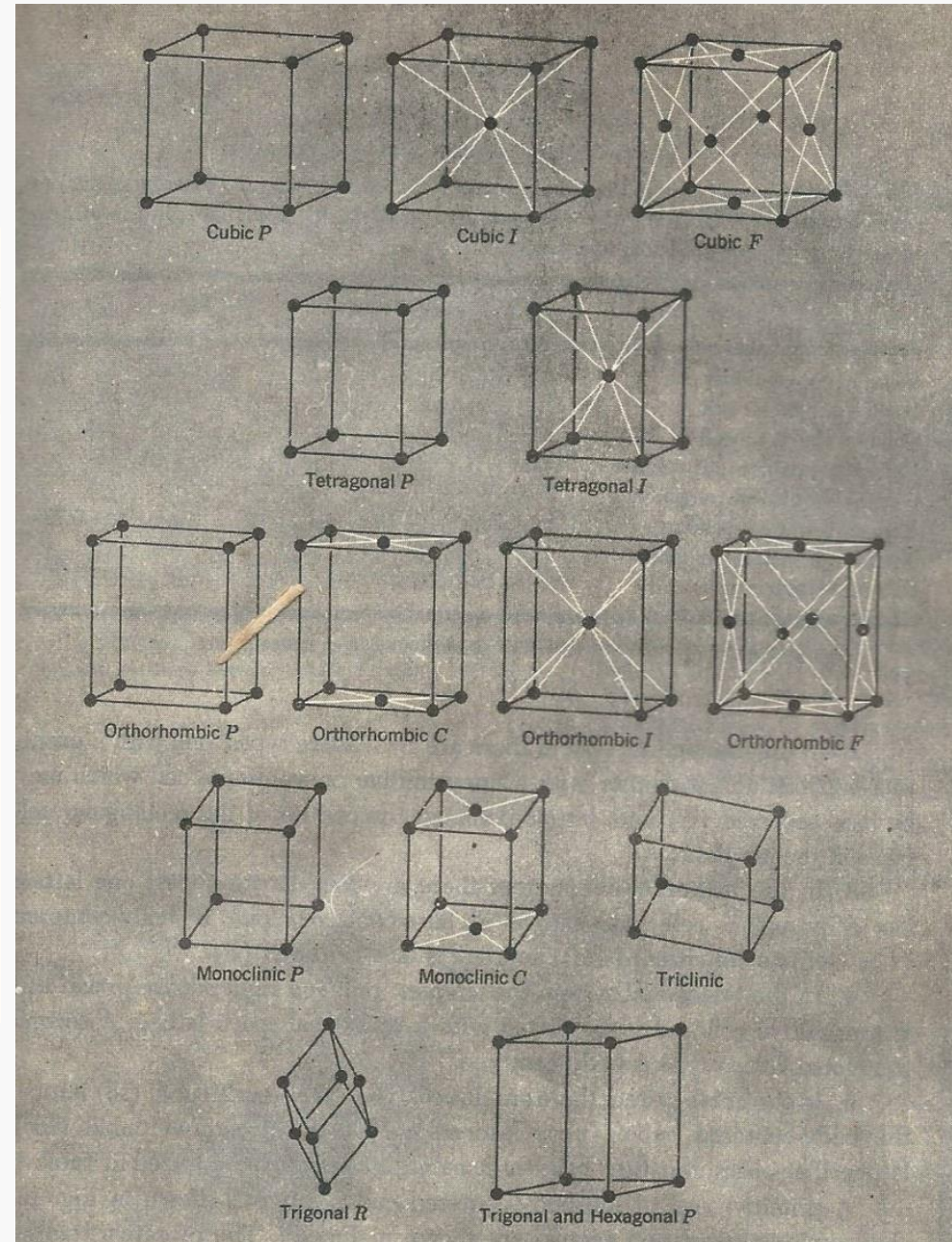
4. Space groups

All symmetry operations which leave a crystal invariant form a group called the space group of the crystal. The space group contains all the translations and the operations of the point group as well as the combinations of the two (screw-rotations and glide reflections). There are 230 space groups in total.

Table 7.1

POINT AND SPACE GROUPS OF BRAVAIS LATTICES AND CRYSTAL STRUCTURES

	BRAVAIS LATTICE (BASIS OF SPHERICAL SYMMETRY)	CRYSTAL STRUCTURE (BASIS OF ARBITRARY SYMMETRY)
Number of point groups:	7 ("the 7 crystal systems")	32 ("the 32 crystallographic point groups")
Number of space groups:	14 ("the 14 Bravais lattices")	230 ("the 230 space groups")

2.3 Reciprocal Lattices

The reciprocal lattice plays a fundamental role in most analytic studies of periodic structures. One is led to it from such diverse avenues as the theory of crystal diffraction, theory of electrons in a crystal, etc.

1. Definition of a reciprocal lattice:

Consider a plane wave $exp(i\mathbf{k} \cdot \mathbf{r})$ in a Bravais lattice . For a general $\mathbf{k}$, such a plane wave will not have the periodicity of the Bravais lattice, but for certain special choices of wave vector, it will.

Definition: The set of all wave vectors $\{\mathbf{G}_m\}$ that yield plane waves with the periodicity of a given Bravais lattice $\{\mathbf{R}_n\}$ is called its reciprocal lattice.

$$\text{If } \mathbf{G} \in \{\mathbf{G}_m\} \text{ of } \{\mathbf{R}_n\}, \; e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R}_n)} = e^{i\mathbf{G}\cdot\mathbf{r}} \text{ for any } \mathbf{r}, \; i.e., e^{i\mathbf{G}\cdot\mathbf{R}_n} = 1.$$

The reciprocal lattice itself is a Bravais lattice $\{\mathbf{G}_m\}$.

The three primitive vectors of the reciprocal lattice $\{\mathbf{G}_m\}$ are

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1.(\mathbf{a}_2 \times \mathbf{a}_3)}, \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1.(\mathbf{a}_2 \times \mathbf{a}_3)}, \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1.(\mathbf{a}_2 \times \mathbf{a}_3)} \ \& \ \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{if};$$

$$\mathbf{G}_m = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3 \ (m_i \text{ are integers}).$$
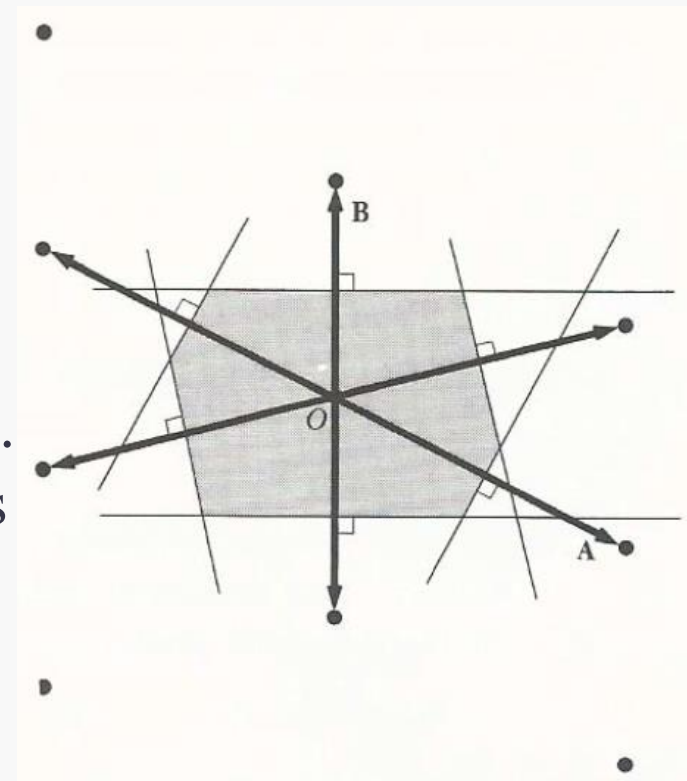
Any vector in the reciprocal space can be written as

$$\mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2 + k_3 \mathbf{b}_3.$$

2. Brillouin zone:
   Definition of (first) Brillouin zone:
   As for a direct lattice, there are many ways to
   construct a primitive cell for a reciprocal lattice.
   The Wigner-Seitz cell of the reciprocal lattice is
   a called the first Brillouin zone or simply the
   Brillouin zone.

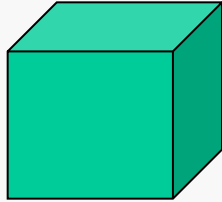# Some examples of reciprocal lattice and first Brillouin zone

a. Simple cubic lattice (sc)

$$\vec{a}_1 = a\hat{i}$$
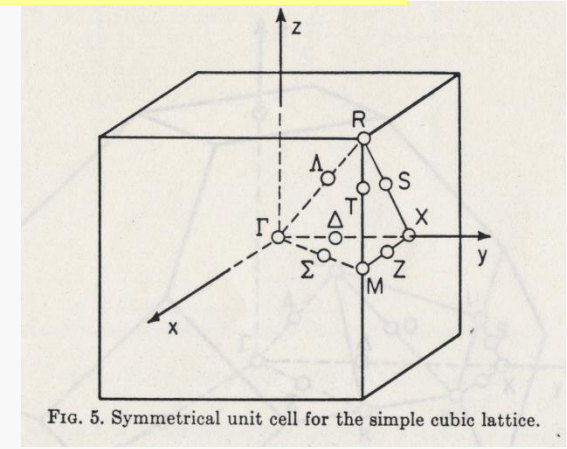
$$\vec{a}_2 = a\hat{j}$$

$$\vec{a}_3 = a\hat{k}$$

Wigner-Seitz cell

$$\vec{b}_1 = \frac{2\pi}{a}\hat{i}$$

$$\vec{b}_2 = \frac{2\pi}{a}\hat{j}$$

$$\vec{b}_3 = \frac{2\pi}{a}\hat{k}$$

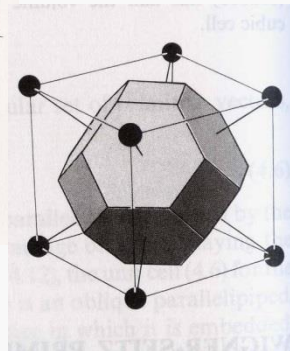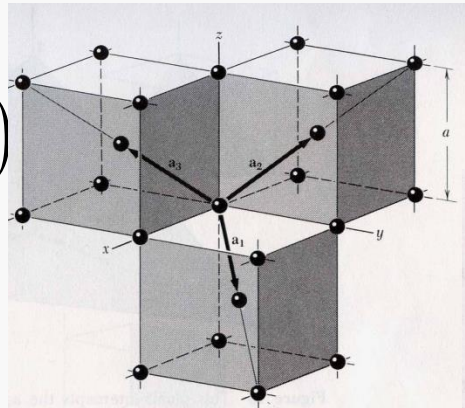FIG. 5. Symmetrical unit cell for the simple cubic lattice.

First Brillouin zone

The reciprocal lattice of a sc lattice is a sc lattice of side $\dfrac{2\pi}{a}$

b. Body center cubic lattice (bcc)

$$\vec{a}_1 = \frac{a}{2}\left(-\vec{i} + \vec{j} + \vec{k}\right)$$

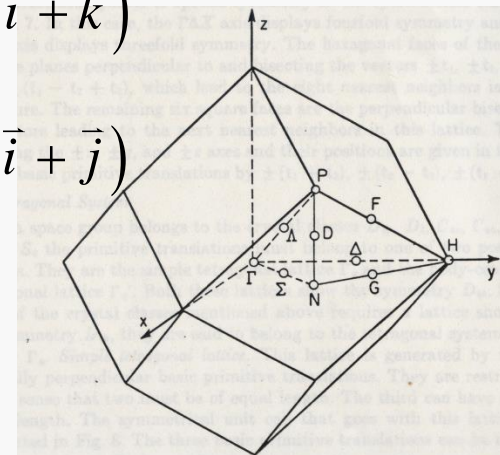$$\vec{a}_2 = \frac{a}{2}\left(\vec{i} - \vec{j} + \vec{k}\right)$$

$$\vec{a}_3 = \frac{a}{2}\left(\vec{i} + \vec{j} - \vec{k}\right)$$

$$\vec{b}_1 = \frac{4\pi}{a}\frac{1}{2}\left(\vec{j} + \vec{k}\right)$$

$$\vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}\left(\vec{i} + \vec{k}\right)$$

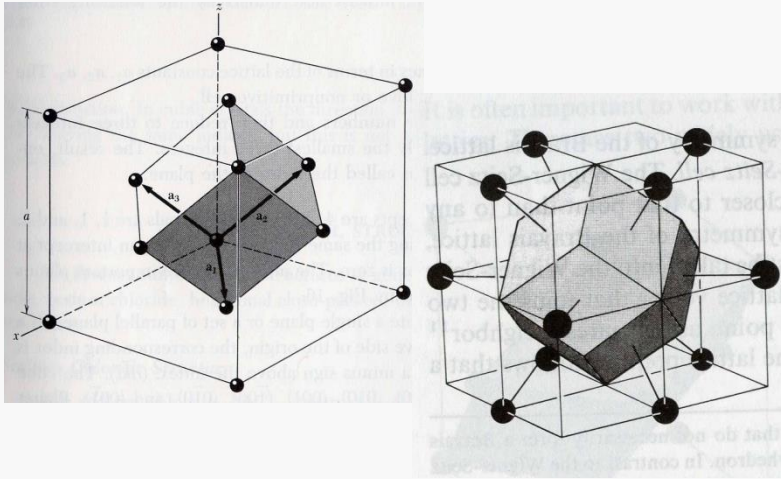$$\vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}\left(\vec{i} + \vec{j}\right)$$

The reciprocal lattice of a bcc lattice is a fcc lattice of side $\dfrac{4\pi}{a}$

FIG. 6. Symmetrical unit cell for the face-centered cubic lattice.

c. Face centered cubic lattice (fcc)

$$\vec{a}_1 = \frac{a}{2}\left(\vec{j} + \vec{k}\right)$$

$$\vec{a}_2 = \frac{a}{2}\left(\vec{i} + \vec{k}\right)$$

$$\vec{a}_3 = \frac{a}{2}\left(\vec{i} + \vec{j}\right)$$

$$\vec{b}_1 = \frac{4\pi}{a}\left(-\vec{i} + \vec{j} + \vec{k}\right)$$

$$\vec{b}_2 = \frac{4\pi}{a}\left(\vec{i} - \vec{j} + \vec{k}\right)$$

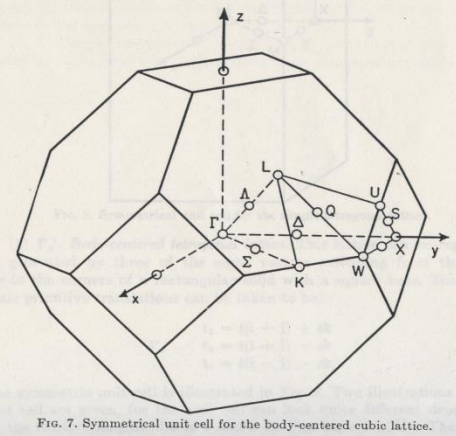$$\vec{b}_3 = \frac{4\pi}{a}\left(\vec{i} + \vec{j} - \vec{k}\right)$$

Fig. 7. Symmetrical unit cell for the body-centered cubic lattice.

1 BZ of a fcc lattice

The reciprocal lattice of a fcc lattice is a bcc lattice of side $\dfrac{4\pi}{a}$

d. Hexagonal lattice (hex)

$$\vec{a}_1 = a\left(\frac{1}{2}\vec{i} + \frac{\sqrt{3}}{2}\vec{j}\right)$$

$$\vec{a}_2 = a\left(\frac{1}{2}\vec{i} - \frac{\sqrt{3}}{2}\vec{j}\right)$$

$$\vec{a}_3 = c\vec{k}$$

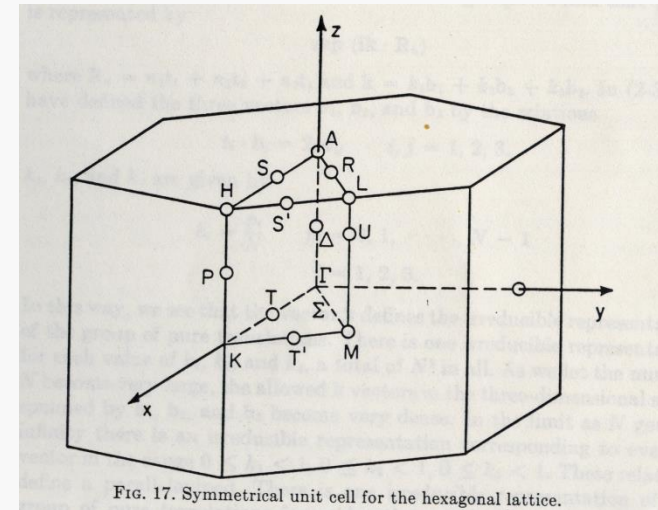Homework: $\vec{b}_1, \vec{b}_2, \vec{b}_3 = ?$

Fig. 17. Symmetrical unit cell for the hexagonal lattice.

3. Extended Brillouin zone:

If, starting from one lattice point as the origin, draw connecting lines to all other G_ms, the planes erected at the mid-points of these lines define the boundaries of the first, second, third, …, Brillouin zones. The **k**-points on the planes exactly satisfy (the Bragg reflection conditions):

$$k^2 = (\mathbf{k} - \mathbf{G}_m)^2.$$

This construction of the extended Brillouin zone is especially useful for any (x-ray, neutron and electron) diffraction experiments. As will be seen in the next chapter, it is also useful in band theory, e.g., in understanding the formation of energy bands in crystals.
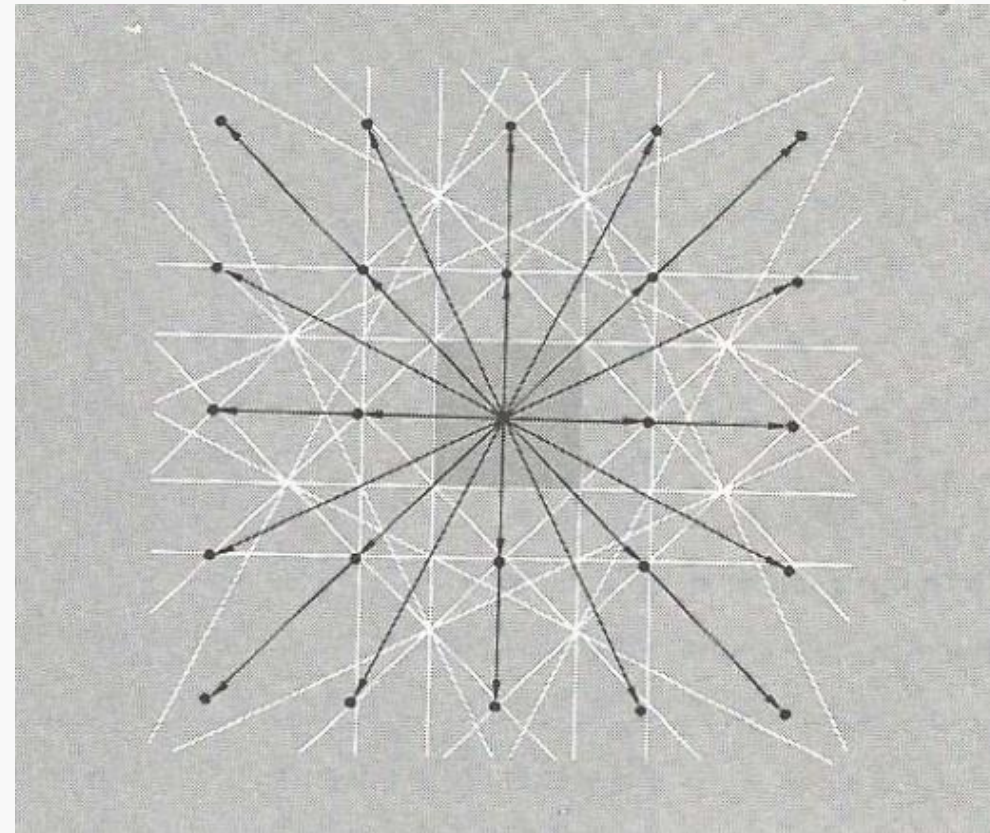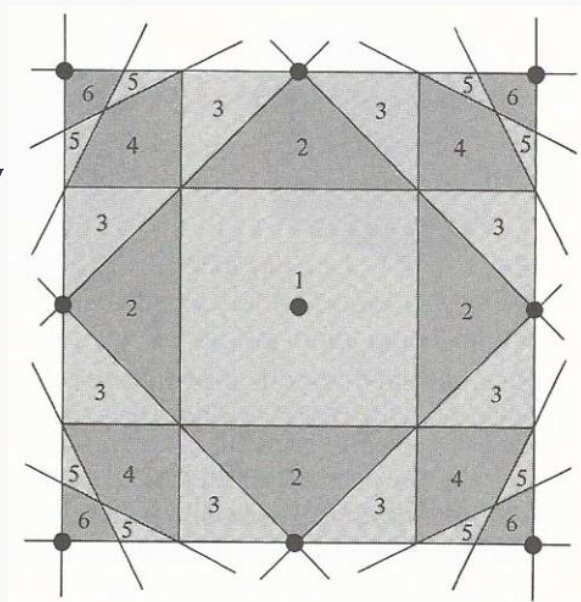
bcc | fcc

1st BZ   I
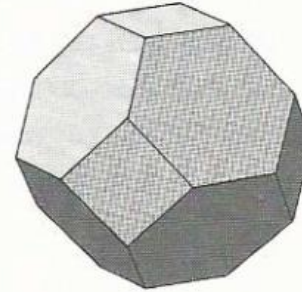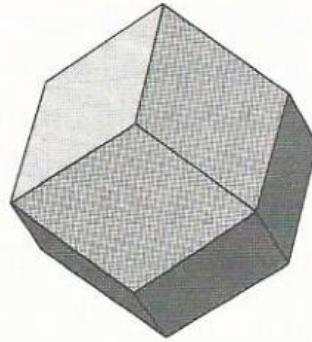
2nd BZ   II
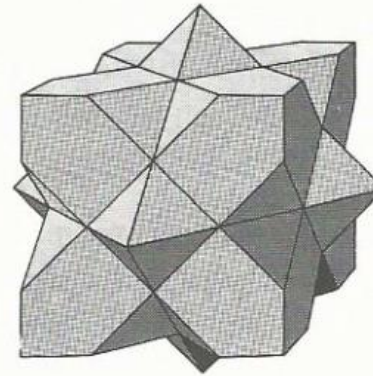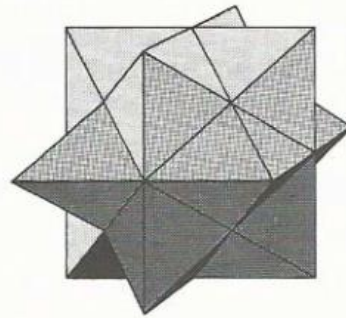
3rd BZ   III
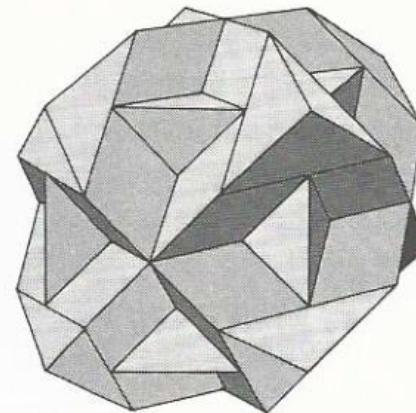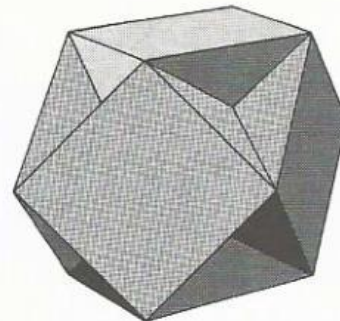
(a)   (b)

2.4 Classification of Bravais Lattices and Crystal Structures

The seven crystal systems:

cubic
(a)

monoclinic
(d)

trigonal
(f)

tetragonal
(b)

triclinic
(e)

orthorhombic
(c)

hexagonal
(g)

The 14 Bravais lattices:

Cubic P

Cubic I

Cubic F

Tetragonal P

Tetragonal I

Orthorhombic P

Orthorhombic C

Orthorhombic I

Orthorhombic F

Monoclinic P

Monoclinic C

Triclinic

Trigonal R

Trigonal and Hexagonal P
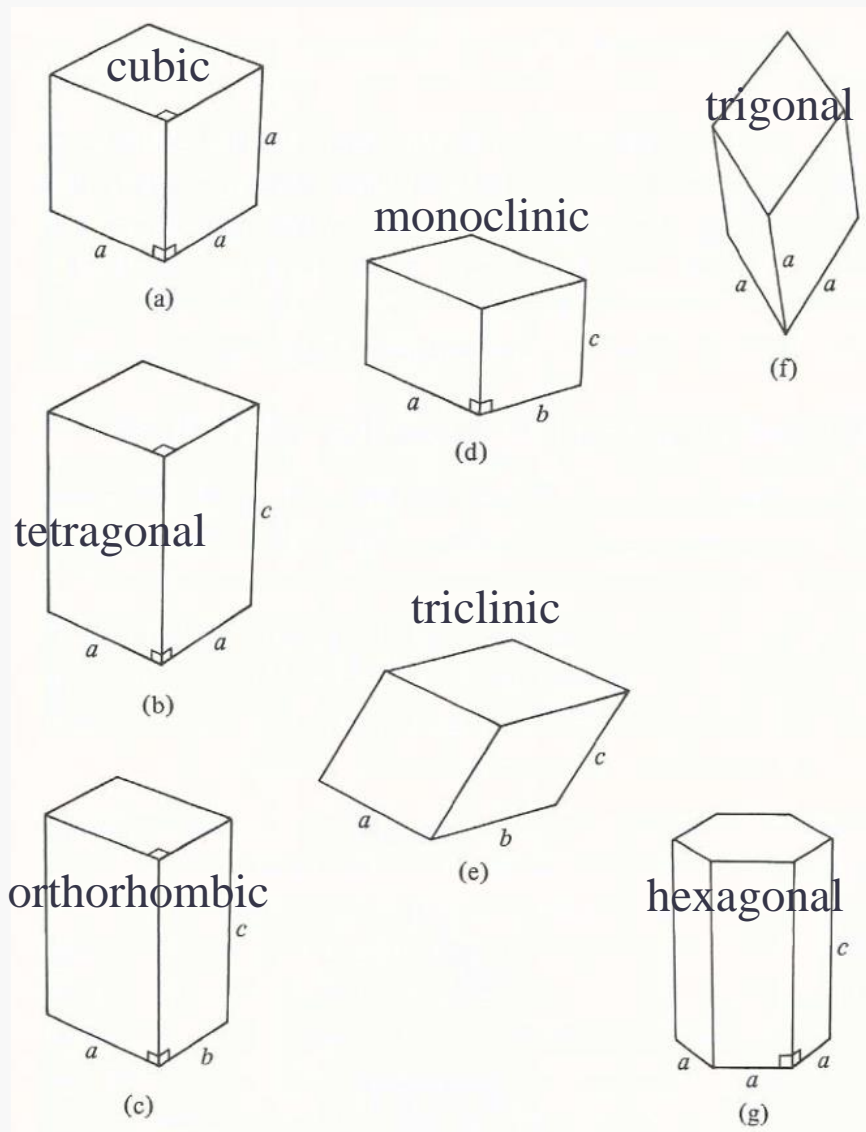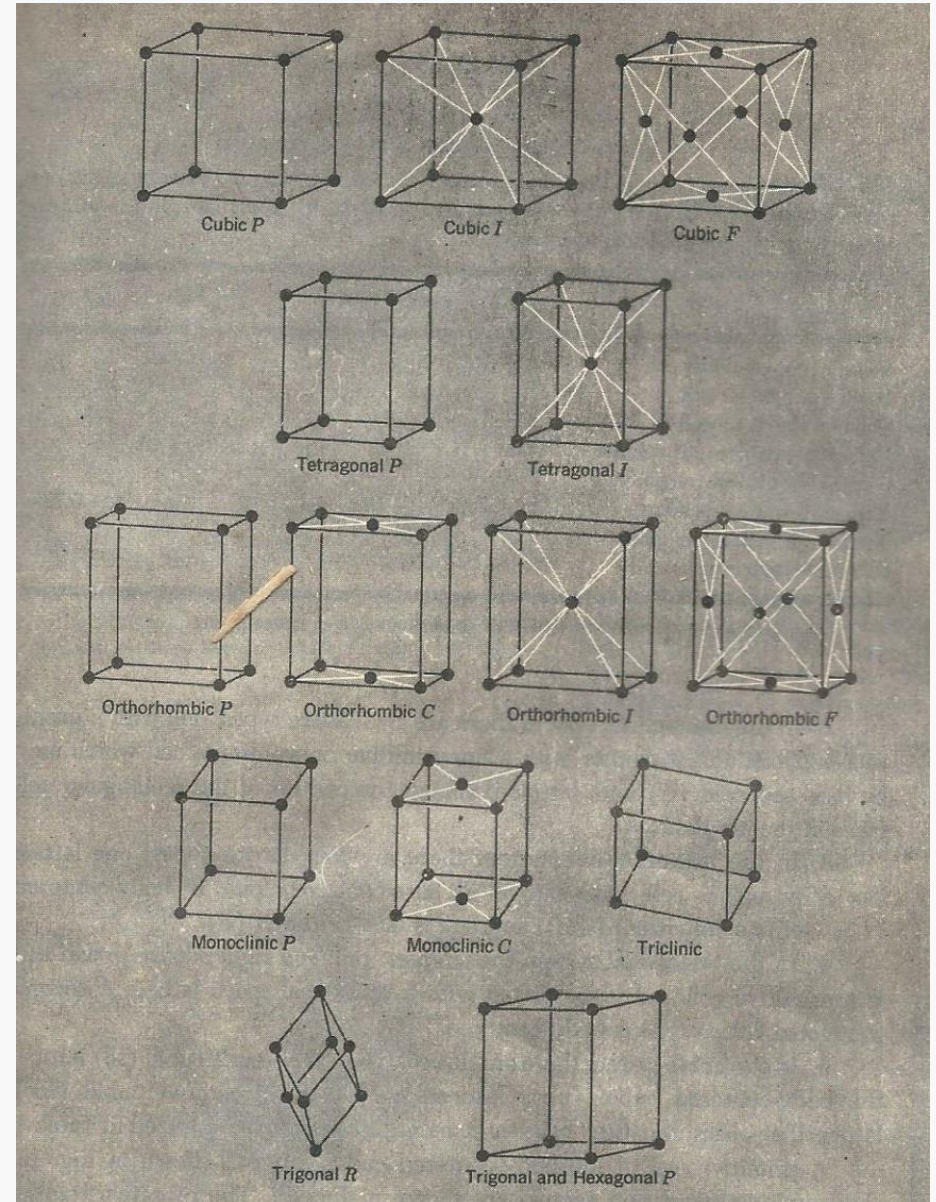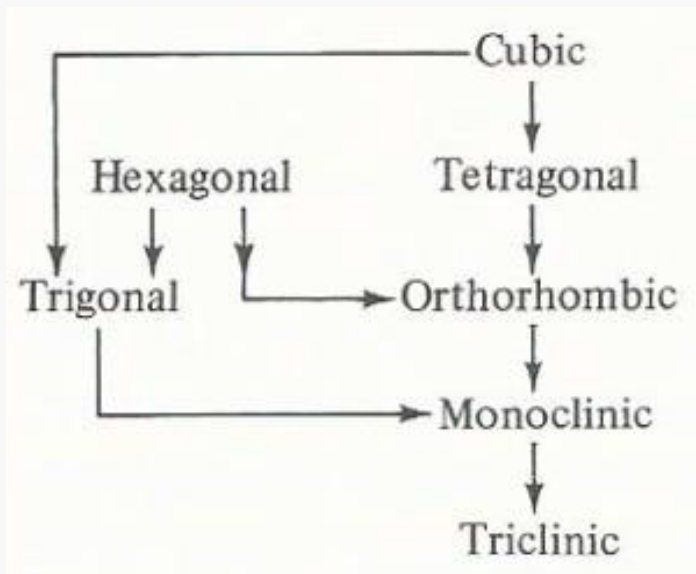
The hierarchy of symmetries among the seven crystal systems.

ENUMERATION OF SOME SIMPLE SPACE GROUPS

SYSTEM	NUMBER OF POINT GROUPS	NUMBER OF BRAVAIS LATTICES	PRODUCT
Cubic	5	3	15
Tetragonal	7	2	14
Orthorhombic	3	4	12
Monoclinic	3	2	6
Triclinic	2	1	2
Hexagonal	7	1	7
Trigonal	5	1	5
Totals	32	14	61

POINT AND SPACE GROUPS OF BRAVAIS LATTICES AND CRYSTAL STRUCTURES

	BRAVAIS LATTICE (BASIS OF SPHERICAL SYMMETRY)	CRYSTAL STRUCTURE (BASIS OF ARBITRARY SYMMETRY)
Number of point groups:	7 ("the 7 crystal systems")	32 ("the 32 crystallographic point groups")
Number of space groups:	14 ("the 14 Bravais lattices")	230 ("the 230 space groups")

The 14 Bravais lattices

Bravails lattice		P	Basic vectors	V
P Triclinic primitive	Γ_t	$\bar{1}\,(C_i)$	arbitrary	$\mathbf{t}_1 \cdot (\mathbf{t}_2 \times \mathbf{t}_3)$
P Monoclinic primitive	Γ_m	$2/m\,(C_{2h})$	$(0,-b,0);(a\sin\gamma,-a\cos\gamma,0);(0,0,c)$	$abc\sin\gamma$
B Monoclinic primitive	Γ_m^b	$2/m\,(C_{2h})$	$(0,-b,0);\frac{1}{2}(a\sin\gamma,-a\cos\gamma,-c);$ $\frac{1}{2}(a\sin\gamma,-a\cos\gamma,c)$	$\frac{1}{2}abc\sin\gamma$
P Orthorhombic primitive	Γ_o	$mmm\,(D_{2h})$	$(0,-b,0);(a,0,0);(0,0,c)$	abc
C Orthorhombic base-centred	Γ_o^b	$mmm\,(D_{2h})$	$\frac{1}{2}(a,-b,0);\frac{1}{2}(a,b,0);(0,0,c)$	$\frac{1}{2}abc$
I Orthorhombic body-centred	Γ_o^v	$mmm\,(D_{2h})$	$\frac{1}{2}(a,b,c);\frac{1}{2}(-a,-b,c);\frac{1}{2}(a,-b,-c)$	$\frac{1}{2}abc$
F Orthorhombic face-centred	Γ_o^f	$mmm\,(D_{2h})$	$\frac{1}{2}(a,0,c);\frac{1}{2}(0,-b,c);\frac{1}{2}(a,-b,0)$	$\frac{1}{4}abc$
P Tetragonal primitive	Γ_q	$4/mmm\,(D_{4h})$	$(a,0,0);(0,a,0);(0,0,c)$	a^2c
P Tetragonal body-centred	Γ_q^v	$4/mmm\,(D_{4h})$	$\frac{1}{2}(-a,a,c);\frac{1}{2}(a,-a,c);\frac{1}{2}(a,a,-c)$	$\frac{1}{2}a^2c$
P Trigonal primitive	Γ_{rh}	$\bar{3}m\,(D_{3d})$	$(0,-a,c);\frac{1}{2}(a\sqrt{3},a,2c);$ $\frac{1}{2}(-a\sqrt{3},a,2c)$	$\frac{1}{2}3\sqrt{3}a^2c$
P Hexagonal primitive	Γ_h	$6/mmm\,(D_{6h})$	$(0,-a,0);\frac{1}{2}(a\sqrt{3},a,0);(0,0,c)$	$\frac{1}{2}\sqrt{3}a^2c$
P Cubic primitive	Γ_c	$m3m\,(O_h)$	$(a,0,0);(0,a,0);(0,0,a)$	a^3
F Cubic face-centred	Γ_c^f	$m3m\,(O_h)$	$\frac{1}{2}(0,a,a);\frac{1}{2}(a,0,a);\frac{1}{2}(a,a,0)$	$\frac{1}{4}a^3$
I Cubic body-centred	Γ_c^v	$m3m\,(O_h)$	$\frac{1}{2}(-a,a,a);\frac{1}{2}(a,-a,a);\frac{1}{2}(a,a,-a)$	$\frac{1}{2}a^3$

Bravais lattice		Reciprocal vectors, g_1, g_2, g_3.	$8\pi^3/V$
Triclinic primitive	Γ_t	arbitrary	$g_1 \cdot (g_2 \times g_3)$
Monoclinic primitive	Γ_m	$2\pi/b(-\cot\gamma, -1, 0)$; $2\pi/a(\text{cosec}\,\gamma, 0, 0)$; $2\pi/c(0, 0, 1)$	$8\pi^3/abc \sin\gamma$
Monoclinic base-centred	Γ_m^b	$2\pi/b(-\cot\gamma, -1, 0)$; $2\pi/ac(c\,\text{cosec}\,\gamma, 0, -a)$; $2\pi/ac(c\,\text{cosec}\,\gamma, 0, a)$	$16\pi^3/abc \sin\gamma$
Orthorhombic primitive	Γ_o	$2\pi/b(0, -1, 0)$; $2\pi/a(1, 0, 0)$; $2\pi/c(0, 0, 1)$	$8\pi^3/abc$
Orthorhombic base-centred	Γ_o^b	$2\pi/ba(b, -a, 0)$; $2\pi/ba(b, a, 0)$; $2\pi/c(0, 0, 1)$	$16\pi^3/abc$
Orthorhombic body-centred	Γ_o^v	$2\pi/ca(c, 0, a)$; $2\pi/cb(0, -c, b)$; $2\pi/ba(b, -a, 0)$	$16\pi^3/abc$
Orthorhombic face-centred	Γ_o^f	$2\pi(1/a, 1/b, 1/c)$; $2\pi(-1/a, -1/b, 1/c)$; $2\pi(1/a, -1/b, -1/c)$	$32\pi^3/abc$
Tetragonal primitive	Γ_q	$2\pi/a(1, 0, 0)$; $2\pi/a(0, 1, 0)$; $2\pi/c(0, 0, 1)$	$8\pi^3/a^2c$
Tetragonal body-centred	Γ_q^v	$2\pi/ca(0, c, a)$; $2\pi/ca(c, 0, a)$; $2\pi/a(1, 1, 0)$	$16\pi^3/a^2c$
Trigonal primitive	Γ_{rh}	$2\pi(0, -2/3a, 1/3c)$; $2\pi(1/\sqrt{(3)}a, 1/3a, 1/3c)$;	
		$\qquad\qquad\qquad\qquad\qquad 2\pi(-1/\sqrt{(3)}a, 1/3a, 1/3c)$	$16\pi^3/3\sqrt{(3)}a^2c$
Hexagonal primitive	Γ_h	$2\pi/a(1/\sqrt{3}, -1, 0)$; $2\pi/a(2/\sqrt{3}, 0, 0)$; $2\pi/c(0, 0, 1)$	$16\pi^3/\sqrt{(3)}a^2c$
Cubic primitive	Γ_c	$2\pi/a(1, 0, 0)$; $2\pi/a(0, 1, 0)$; $2\pi/a(0, 0, 1)$	$8\pi^3/a^3$
Cubic face-centred	Γ_c^f	$2\pi/a(-1, 1, 1)$; $2\pi/a(1, -1, 1)$; $2\pi/a(1, 1, -1)$	$32\pi^3/a^3$
Cubic body-centred	Γ_c^v	$2\pi/a(0, 1, 1)$; $2\pi/a(1, 0, 1)$; $2\pi/a(1, 1, 0)$	$16\pi^3/a^3$

Notes to Table 3.3

(i) Column 1 lists the Bravais lattice of the translation group, T, in direct space. The basic vectors of the Bravais lattices are given in Table 3.1.

(ii) Column 2 lists the coordinates of the translations g_1, g_2, and g_3 of reciprocal space with respect to the k_x, k_y, k_z axes. For example, $g_1 = (p, q, r)$ means that $g_1 = p\mathbf{l} + q\mathbf{m} + r\mathbf{n}$, where l, m, and n are unit vectors in the k_x, k_y, and k_z directions.

(iii) Column 3 gives $(8\pi^3/V)$, the volume of the Brillouin zone.

(see Appendix A for all the Brillouin zones for the 14 Bravais lattices.)