

Table 1.1 Relative Abundance of Elements in the Universe

Element	Relative Abundance (Si = 1)
Hydrogen (H)	12,000
Helium (He)	2,800
Oxygen (O)	16
Nitrogen (N)	8
Carbon (C)	3
Iron (Fe)	2.6
Silicon (Si)	1
Magnesium (Mg)	0.89
Sulfur (S)	0.33
Nickel (Ni)	0.21
Aluminum (Al)	0.09
Calcium (Ca)	0.07
Sodium (Na)	0.045
Chlorine (Cl)	0.025

Table 1.2 Relative Abundance of Selected Elements in the Earth's Crust

Element	Relative Abundance (ppm)	Element	Relative Abundance (ppm)
Oxygen (O)	466,000	Fluorine (F)	300
Silicon (Si)	277,200	Strontium (Sr)	300
Aluminum (Al)	81,300	Barium (Ba)	250
Iron (Fe)	50,000	Zirconium (Zr)	220
Calcium (Ca)	36,300	Chromium (Cr)	200
Sodium (Na)	28,300	Vanadium (V)	150
Potassium (K)	25,900	Zinc (Zn)	132
Magnesium (Mg)	20,900	Nickel (Ni)	80
Titanium (Ti)	4,400	Molybdenum (Mo)	15
Hydrogen (H)	1,400	Uranium (U)	4
Phosphorus (P)	1,180	Mercury (Hg)	0.5
Manganese (Mn)	1,000	Silver (Ag)	0.1
Sulfur (S)	520	Platinum (Pt)	0.005
Carbon (C)	320	Gold (Au)	0.005
Chlorine (Cl)	314	Helium (He)	0.003

1 H	
3 Li	4 Be
11 Na	12 Mg
19 K	20 Ca
37 Rb	38 Sr
55 Cs	56 Ba
87 Fr	88 Ra

Temperature: 290 °K
16 °C
62 °F

21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn
39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd
57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg
89 Ac									

5 B	6 C	7 N	8 O	9 F	10 Ne
13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn

Legend

- Solid
- Liquid
- Gas
- Not Available

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

1 H	
3 Li	4 Be
11 Na	12 Mg
19 K	20 Ca
37 Rb	38 Sr
55 Cs	56 Ba
87 Fr	88 Ra

Temperature: 1280 °K
 1006 °C
 1844 °F

21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn
39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd
57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg
89 Ac									

2 He									
5 B	6 C	7 N	8 O	9 F	10 Ne				
13 Al	14 Si	15 P	16 S	17 Cl	18 Ar				
31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr				
49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe				
81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn				

Legend

- Solid
- Liquid
- Gas
- Not Available

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

(b)

1	H
3	4
Li	Be
11	12
Na	Mg
19	20
K	Ca
37	38
Rb	Sr
55	56
Cs	Ba
87	88
Fr	Ra

Temperature: 2280 °K
2006 °C
3644 °F

21	22	23	24	25	26	27	28	29	30
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
39	40	41	42	43	44	45	46	47	48
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
57	72	73	74	75	76	77	78	79	80
La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
89									
Ac									

5	6	7	8	9	10
B	C	N	O	F	Ne
13	14	15	16	17	18
Al	Si	P	S	Cl	Ar
31	32	33	34	35	36
Ga	Ge	As	Se	Br	Kr
49	50	51	52	53	54
In	Sn	Sb	Te	I	Xe
81	82	83	84	85	86
Tl	Pb	Bi	Po	At	Rn

Legend

- Solid
- Liquid
- Gas
- Not Available

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

(c)

1	H
3	4
Li	Be
11	12
Na	Mg
19	20
K	Ca
37	38
Rb	Sr
55	56
Cs	Ba
87	88
Fr	Ra

Temperature: 3780 °K
3506 °C
6344 °F

21	22	23	24	25	26	27	28	29	30
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
39	40	41	42	43	44	45	46	47	48
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
57	72	73	74	75	76	77	78	79	80
La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
89									
Ac									

5	6	7	8	9	10
B	C	N	O	F	Ne
13	14	15	16	17	18
Al	Si	P	S	Cl	Ar
31	32	33	34	35	36
Ga	Ge	As	Se	Br	Kr
49	50	51	52	53	54
In	Sn	Sb	Te	I	Xe
81	82	83	84	85	86
Tl	Pb	Bi	Po	At	Rn

Legend

- Solid
- Liquid
- Gas
- Not Available

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

(d)

Table 1.3 Electronic Structure and Melting Points of the Elements

Source: Ball, Courtney Wulf, Introduction to Materials Science and Engineering, Wiley, 1976

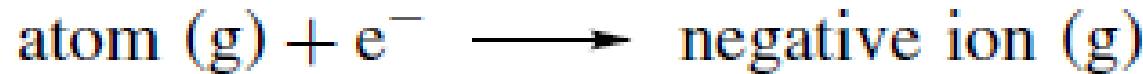
First Ionization Energy (IE).



$$IE = \frac{13.6Z^2}{n^2}$$

where Z is the effective nuclear charge and n is the principal quantum number.

Electron Affinity (EA).



Electronegativity.

$$\chi = \frac{IE + EA}{2}$$

$$\chi = \frac{0.31(n + 1 \pm c)}{r} + 0.5$$

Mulliken's scale

**Pauling's
modified scale or
Gordy's scale**

n: number of valence electrons

c: formal valence charge on the atom with corresponding sign

r: covalent radius

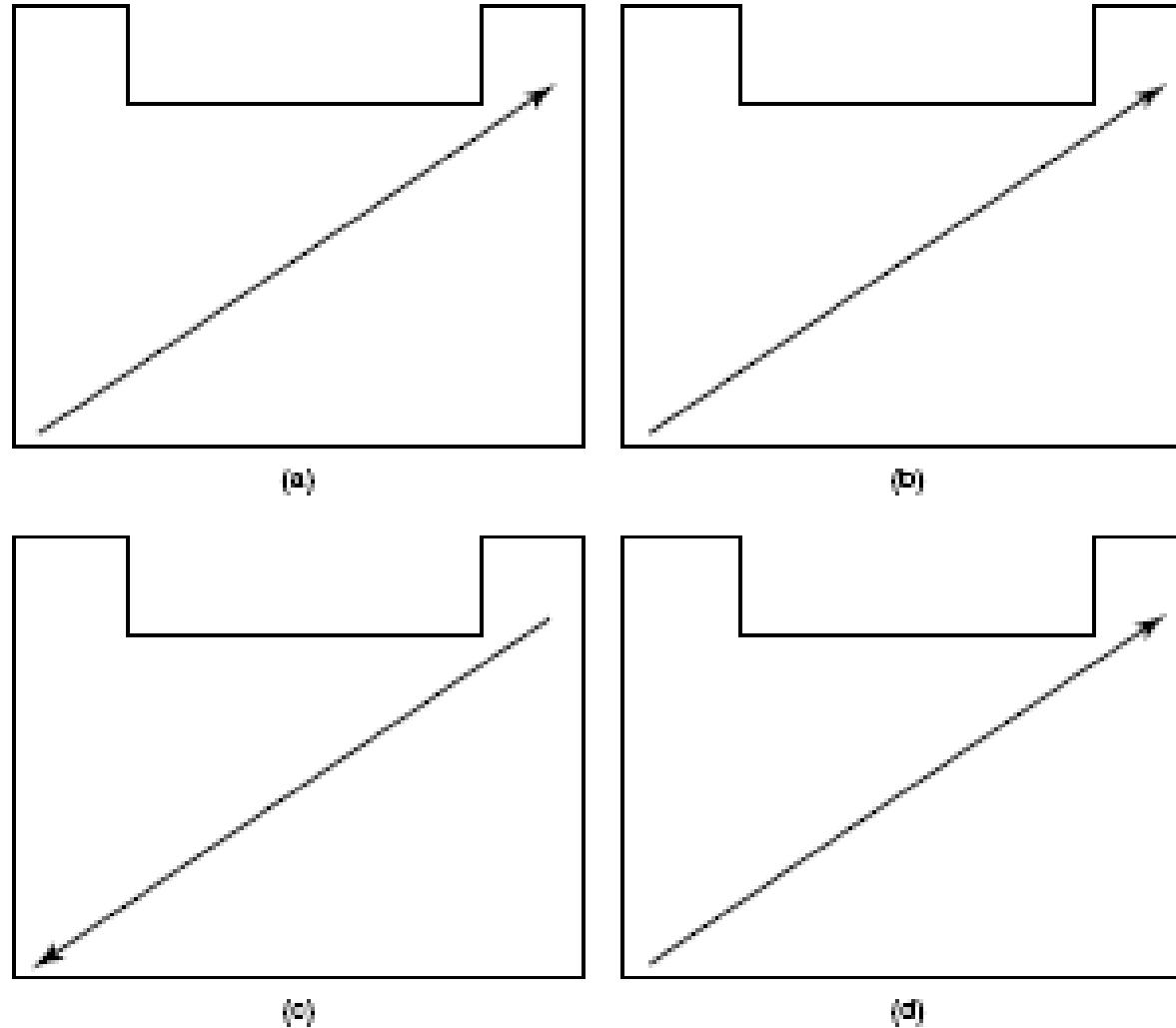


Figure 1.2 Some important trends in the periodic table for (a) ionization energy, (b) electron affinity, (c) atomic and ionic radii, and (d) electronegativity. Increasing values are in the direction of the arrow.

Table 1.4 Ionization Energies, Electron Affinities, and Electronegativities of the Elements

Table 2. Estimated effects of the $\Delta\Delta$ as expressed in kilobarcycles. $1\text{ k}\Omega = 10^{-3}\text{ kilobars}$.

Source: R. H. Dickenson, H. B. Gray, and G. P. Height, *Chemical Principles*, 3rd ed., Pearson Education, Inc., 1979.

Pauling's scale

excess binding energy

$$\Delta_{A-B} = 96.5(\chi_A - \chi_B)^2$$

(kJ/mol)

bond dissociation energy

$$\Delta_{A-B} = DE_{AB} - [(DE_{AA})(DE_{BB})]^{1/2}$$

$$DE_{AB} = [(DE_{AA})(DE_{BB})]^{1/2} + 96.5 (\chi_A - \chi_B)^2$$

(kJ/mol)

Original paper gives $23 (\chi_A - \chi_B)^2$
But units are kcal/mol

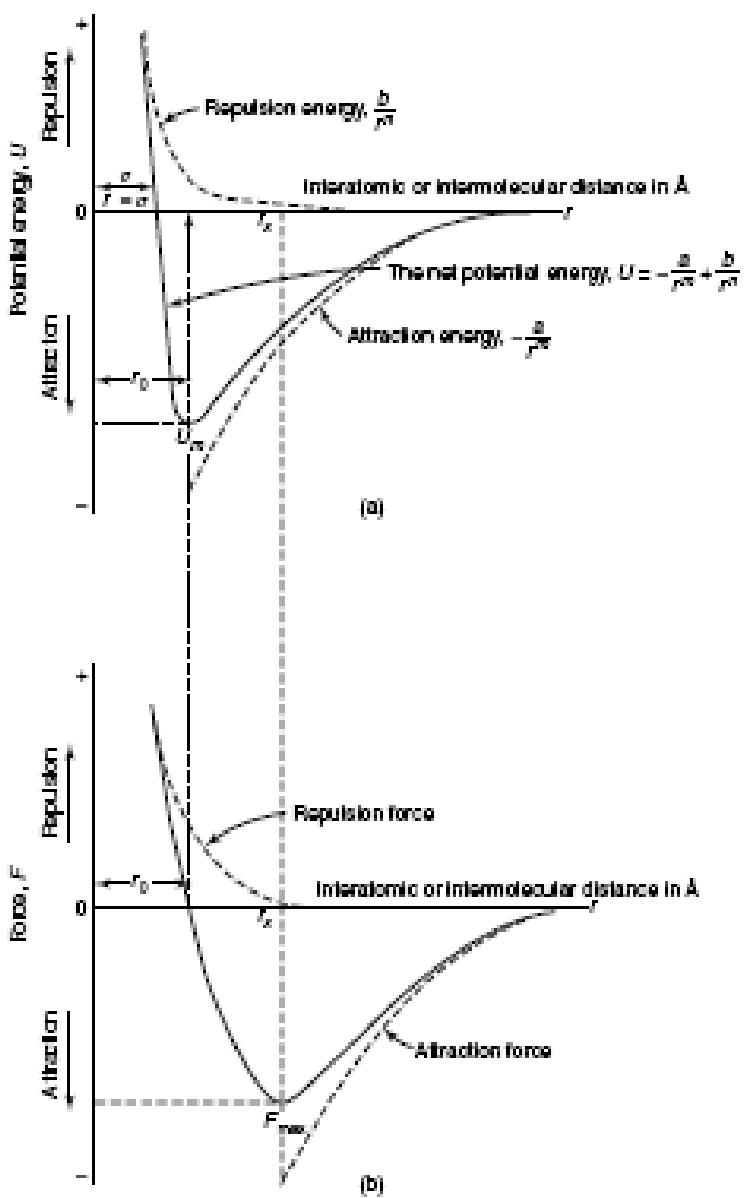


Figure 1.3 The interatomic (a) potential energy and (b) force diagrams. From Z. Jastrzebski, *The Nature and Properties of Engineering Materials*, 2nd ed. by Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

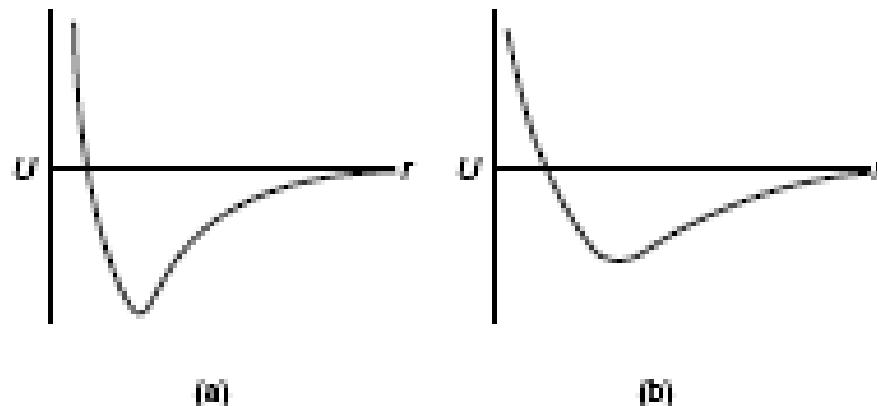


Figure 1.4 Schematic representation of the relationship between the shape of the potential energy well and selected physical properties. Materials with a deep well (a) have a high melting point, high elastic modulus, and low thermal expansion coefficient. Those with a shallow well (b) have a low melting point, low elastic modulus, and high thermal expansion coefficient. Adapted from C. R. Barrett, W. D. Nix, and A. S. Tetelman, *The Principles of Engineering Materials*. Copyright © 1973 by Prentice-Hall, Inc.

BONDING

- Cohesive forces-atoms held together.

Interatomic bonds

Primary
Ionic
Covalent
Metallic

Secondary
Hydrogen
Van der Waals
forces

Material bonding	Bond energy (kcal/mol)
Metallic bonds	27-83
Covalent bonds	15-170
Ionic bonds	140-250
Hydrogen bonds	1-12
van der Waals	1-10

Two atoms are close enough for their atomic orbitals to mix.

The electronegativity values for the two atoms are...

Similar

Very different

Ionic Bonding

The atoms are classified as...

Metals

Nonmetals

Metallic Bonding

Covalent Bonding

The electronegativity values are...

Very close

Different

Nonpolar Covalent

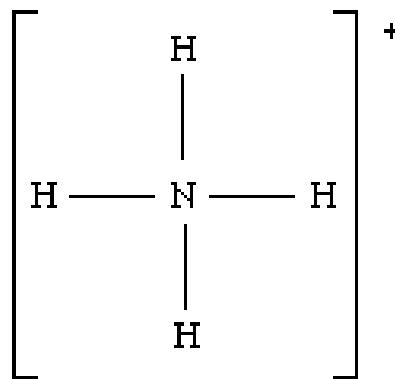
Polar Covalent

increasing electronegativity difference between bonding atoms

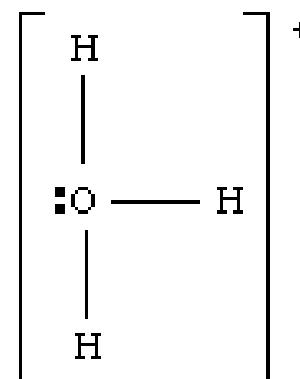
Electronegativity difference	0 - 0.4	0.5 - 2.0	> 2.0
Bond type	nonpolar covalent	polar covalent	ionic
Element types	nonmetal-nonmetal	nonmetal-nonmetal	metal-nonmetal
Examples	H—H Cl—Cl	H—Cl	Na ⁺ Cl ⁻

Coordinate Covalent

A coordinate covalent bond (also called a dative bond) is formed when one atom donates both of the electrons to form a single covalent bond. These electrons originate from the donor atom as an unshared pair.



Ammonium (NH_4^+)



Hydronium (H_3O^+)

Both the ammonium ion and hydronium ion contain one coordinate covalent bond each. A lone pair on the oxygen atom in water contributes two electrons to form a coordinate covalent bond with a hydrogen ion to form the hydronium ion. Similarly, a lone pair on nitrogen contributes 2 electrons to form the ammonium ion. All of the bonds in these ions are indistinguishable once formed, however.

Table 1.5 Examples of Substances with Different Types of Interatomic Bonding

Type of Bond	Substance	Bond Energy, kJ/mol	Melting Point, °C	Characteristics
Ionic	CaCl	651	646	Low electrical conductivity,
	NaCl	768	801	transparent, brittle, high melting point
	LiF	1008	870	
	CuF ₂	2591	1360	
	Al ₂ O ₃	15,192	3500	
Covalent	Ge	315	968	Low electrical conductivity,
	GaAs	~315	1238	very hard, very high melting point
	Si	353	1420	
	SiC	1188	2600	
	Diamond	714	3550	
Metallic	Na	109	97.5	High electrical and thermal conductivity, easily deformable, opaque
	Al	311	660	
	Cu	340	1083	
	Fe	407	1535	
	W	844	3370	
van der Waals	Ne	2.5	-248.7	Weak binding, low melting and boiling points, very compressible
	Ar	7.6	-189.4	
	CH ₄	10	-184	
	Kr	12	-157	
	Cl ₂	31	-103	
Hydrogen bonding	HF	29	-92	Higher melting point than van der Waals bonding, tendency to form groups of many molecules
	H ₂ O	50	0	

$$\% \text{ ionic character} = 100(1 - \exp[-0.25(\chi_A - \chi_B)^2])$$

$$U_A = -\frac{a}{r^m}$$

m has a value of 1 for ions and 6 for molecules.

$$U_R = \frac{b}{r^n}$$

Table 1.6 Values of the Repulsion Exponent

Noble Gas Ion Core	Outer Core Configuration	<i>n</i>
He	$1s^2$	5
Ne	$2s^2 2p^6$	7
Ar	$3s^2 3p^6$	9
Kr	$3d^{10} 4s^2 4p^6$	10
Xe	$4d^{10} 5s^2 5p^6$	12

$$U = U_A + U_R = \frac{-a}{r^m} + \frac{b}{r^n}$$

$$U = -\frac{a}{r^6} + \frac{b}{r^{12}} \quad \text{Lennard-Jones potential}$$

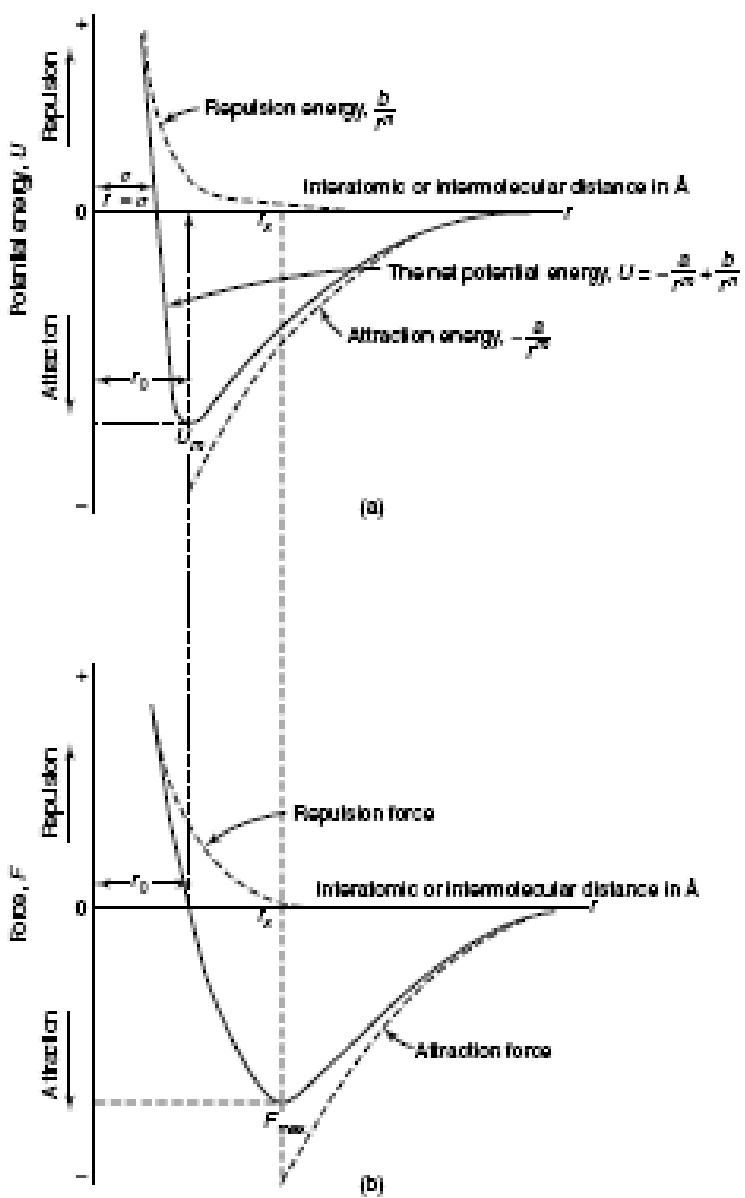


Figure 1.3 The interatomic (a) potential energy and (b) force diagrams. From Z. Jastrzebski, *The Nature and Properties of Engineering Materials*, 2nd ed. by Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

$$F = -\frac{dU}{dr}$$

$$F = -\frac{dU}{dr} = 0, \quad \text{at } r = r_0 \quad \textit{Minimum potential energy}$$

$$F_{\max} = \frac{dF}{dr} = -\frac{d^2U}{dr^2} = 0 \quad \textit{maximum attractive force}$$

$$r_0 = \left(\frac{nb}{ma}\right)^{\frac{1}{n-m}}$$

The Ionic Bond.

$$U = U_A + U_R + \Delta E_{ions}$$

$$U_0 = U_{A,0} + U_{R,0} + \Delta E_{ions} \quad \text{equilibrium potential energy, } U_0$$

Consider formation of NaCl

$$IE = 498 \text{ kJ/mol}$$

For sodium

$$EA = -354 \text{ kJ/mol}$$

For chlorine

$$\Delta E_{ions} = IE_{Na} + EA_{Cl} = 498 - 354 = 144 \text{ kJ/mol}$$

$$F_A = (Z_1 e \times Z_2 e) / (4\pi \varepsilon_0 r^2)$$

$$F_A = +e^2 / (4\pi \varepsilon_0 r^2)$$

$$U_{A,0} = - \int_{\infty}^{r_0} F_A \ dr = e^2 / (4\pi \varepsilon_0 r_0)$$

$$U_{R,0} = e^2 / (4\pi \varepsilon_0 n r_0)$$

$$U_0 = \frac{-e^2}{4\pi \varepsilon_0 r_0} + \frac{e^2}{4\pi \varepsilon_0 n r_0} + \Delta E_{ions}$$

$$U_0 = \left(1 - \frac{1}{n}\right) \left(\frac{-e^2}{4\pi \varepsilon_0 r_0}\right) + \Delta E_{ions}$$

$$r_0 = \left(\frac{nb}{ma}\right)^{\frac{1}{n-m}}$$

Equilibrium bond length
(m=1 and n=8)

$$U_0 = \left(1 - \frac{1}{8}\right) \left[\frac{1(1.6 \times 10^{-19} \text{ C})^2(6.02 \times 10^{23} \text{ mol}^{-1})}{4\pi(8.854 \times 10^{-12} \text{ C}^2/\text{N} \cdot \text{m}^2)(2.36 \times 10^{-10} \text{ m})} \right] + 142$$

$$U_0 = -371 \text{ kJ/mol}$$

Madelung constant, α_M

Taking into account interactions with adjacent atoms that result in an increased interionic spacing compared to an isolated atom.

Depends on the structure of the ionic crystal, the charge on the ions, and the relative size of the ions.

$$U_L = \left(\alpha_M - \frac{1}{n} \right) \left(\frac{-e^2}{4\pi\epsilon_0 r_0} \right) + \Delta E_{ions}$$

For NaCl, $\alpha_M = 1.75$

$$U_L = -811 \text{ kJ/mol}$$

Table 1.7 Typical Values for the Madelung Constant

Compound	Crystal Lattice (see Section 1.1.1)	α_M
NaCl	FCC	1.74756
CsCl	CsCl	1.76267
CaF ₂	Cubic	2.51939
CdCl ₂	Hexagonal	2.244
MgF ₂	Tetragonal	2.381
ZnS (wurtzite)	Hexagonal	1.64132
TiO ₂ (rutile)	Tetragonal	2.408
β -SiO ₂	Hexagonal	2.2197

CRYSTAL STRUCTURE

Point groups

The crystallographic point group or *crystal class* is the mathematical group comprising the symmetry operations that leave at least one point unmoved and that leave the appearance of the crystal structure unchanged.

Symmetry operations include:

Reflection, which reflects the structure across a *reflection plane*

Rotation, which rotates the structure a specified portion of a circle about a *rotation axis*

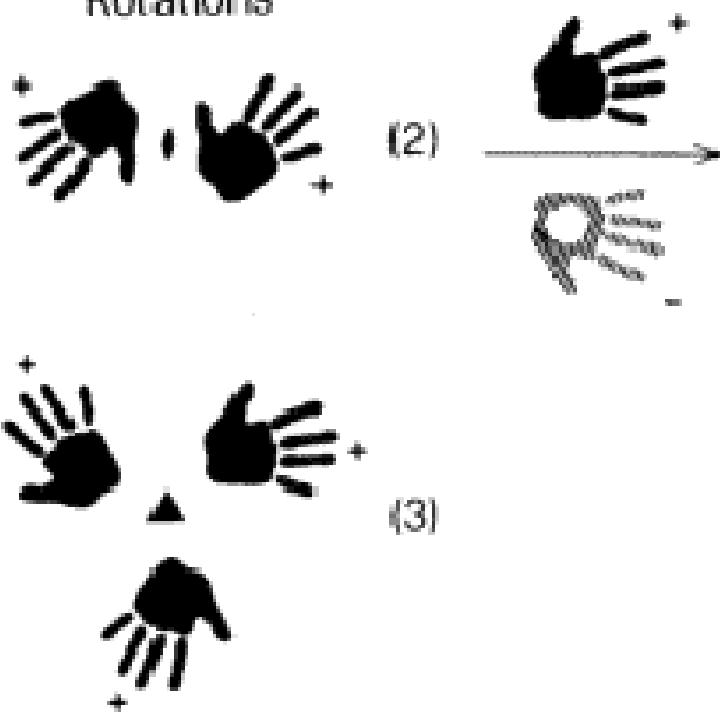
Inversion, which changes the sign of the coordinate of each point with respect to a *center of symmetry* or *inversion point*

Improper rotation, which consists of a rotation about an axis followed by an inversion.

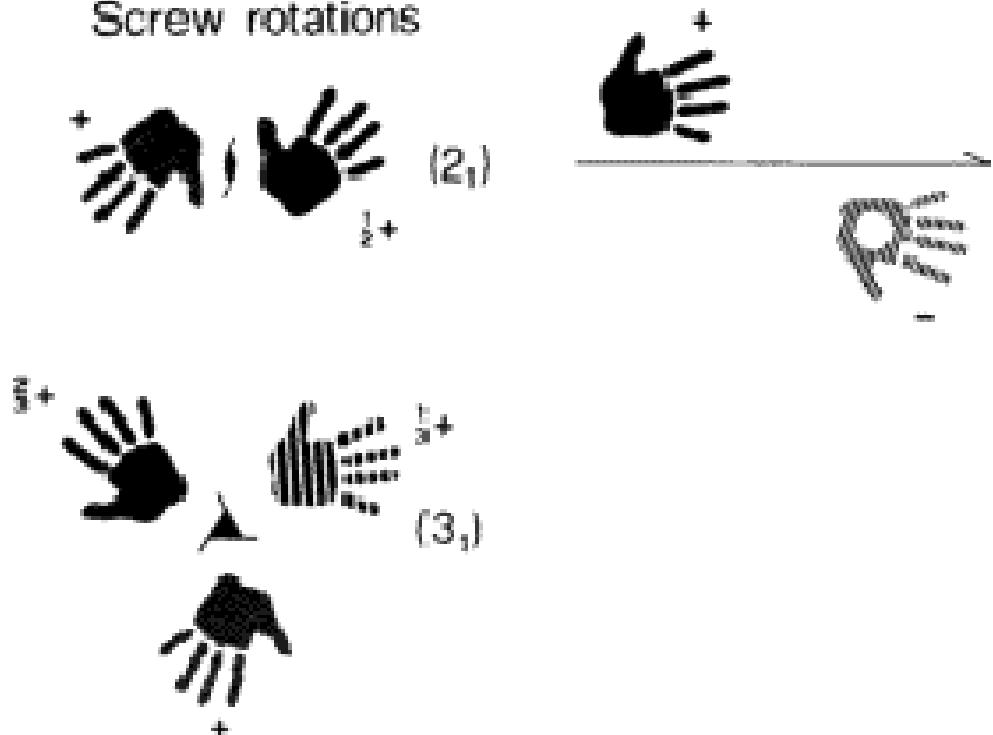
Rotation axes (proper and improper), reflection planes, and centers of symmetry are collectively called *symmetry elements*. There are 32 possible crystal classes.

Each one can be classified into one of the seven crystal systems.

Rotations



Screw rotations

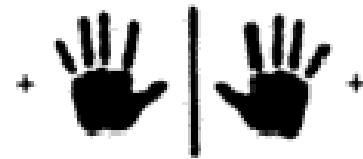


Inversion



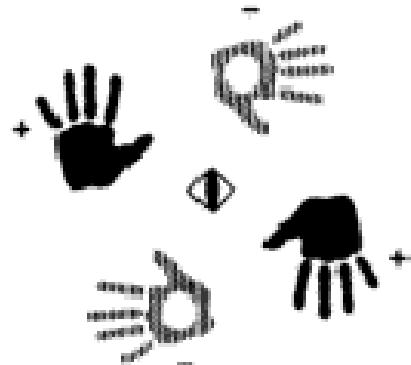
(f)

Reflection



(m)

Rotatory inversion



Axial glide



(a or b)



(c)



Diagonal glide



(n)



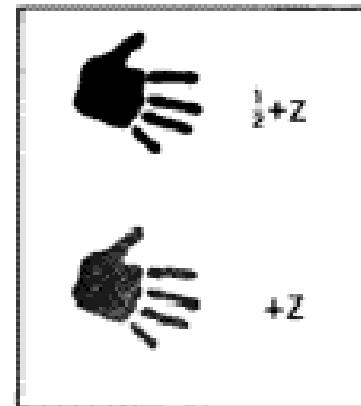
palm up

(indicated by coin)

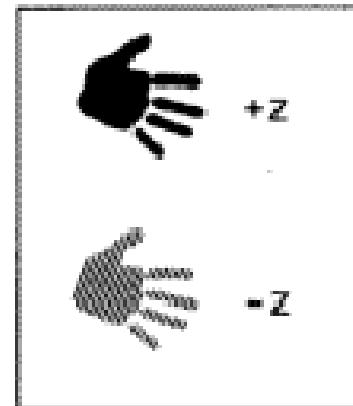


palm down

z-coordinate indicated by darkness of figure as follows



or



Space groups

In addition to the operations of the point group, the space group of the crystal structure contains translational symmetry operations.

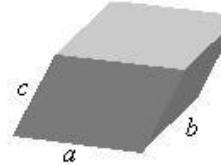
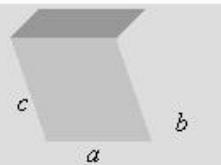
These include:

Pure *translations*, which move a point along a vector

Screw axes, which rotate a point around an axis while translating parallel to the axis.

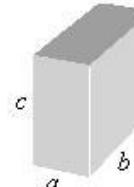
Glide planes, which reflect a point through a plane while translating it parallel to the plane.

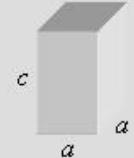
There are 230 distinct space groups.

System	Restrictions	Illustration
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ, \beta > 90^\circ$	

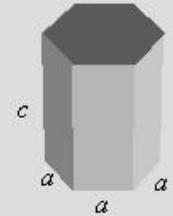
Crystal systems

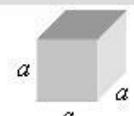
A **crystal system** is a class of point groups.

Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	
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Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	
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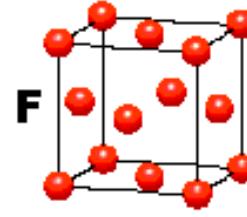
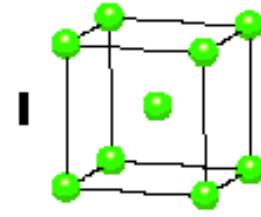
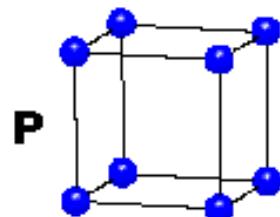
Trigonal (Rhombohedral)	$a = b = c$ $\alpha = \beta = \gamma$	
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Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
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Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	
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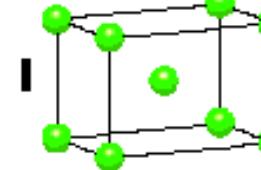
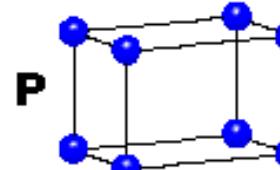
CUBIC

$a = b = c$
 $\alpha = \beta = \gamma = 90^\circ$



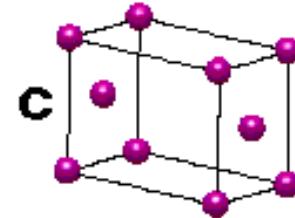
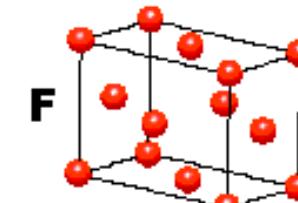
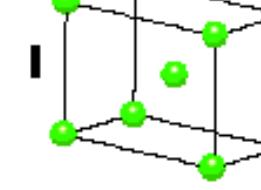
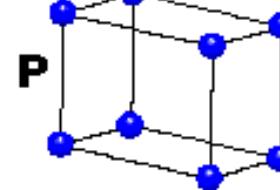
TETRAGONAL

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



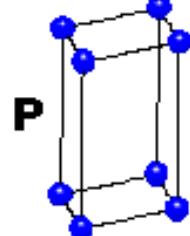
ORTHORHOMBIC

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



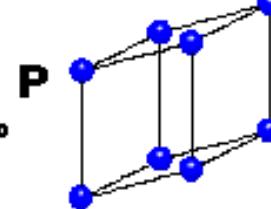
HEXAGONAL

$a = b \neq c$
 $\alpha = \beta = 90^\circ$
 $\gamma = 120^\circ$



TRIGONAL

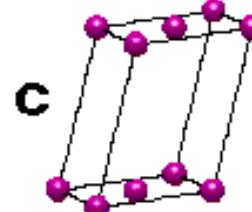
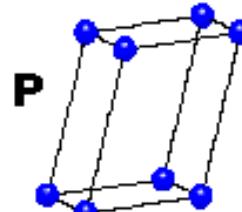
$a = b = c$
 $\alpha = \beta = \gamma \neq 90^\circ$



(Rhombohedral)

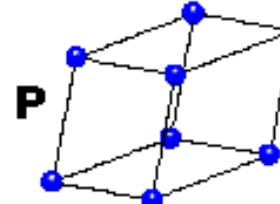
MONOCLINIC

$a \neq b \neq c$
 $\alpha = \gamma = 90^\circ$
 $\beta \neq 120^\circ$



TRICLINIC

$a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$



4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

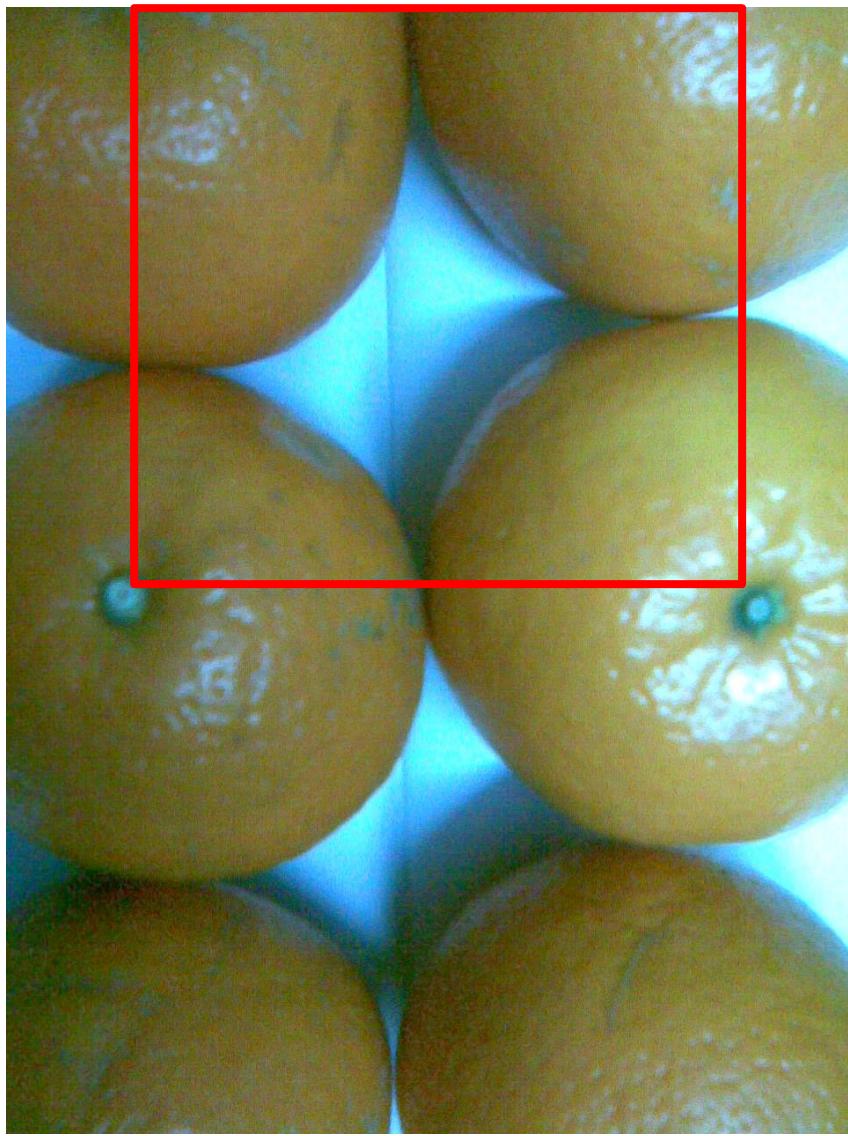
C = Side-Centred

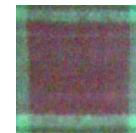
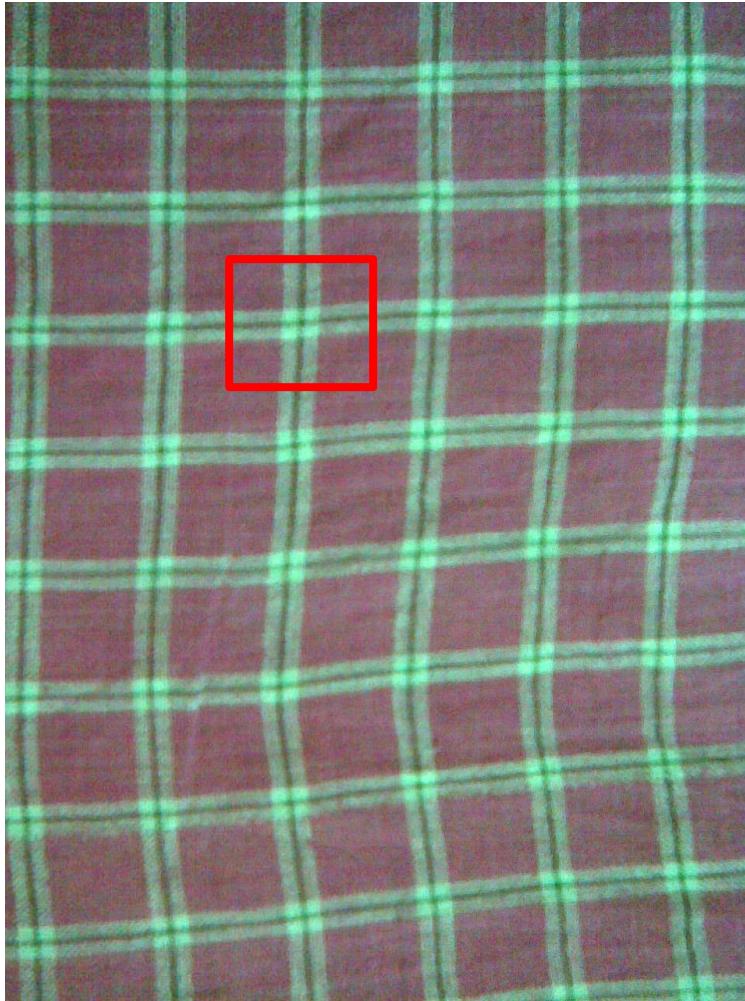
+

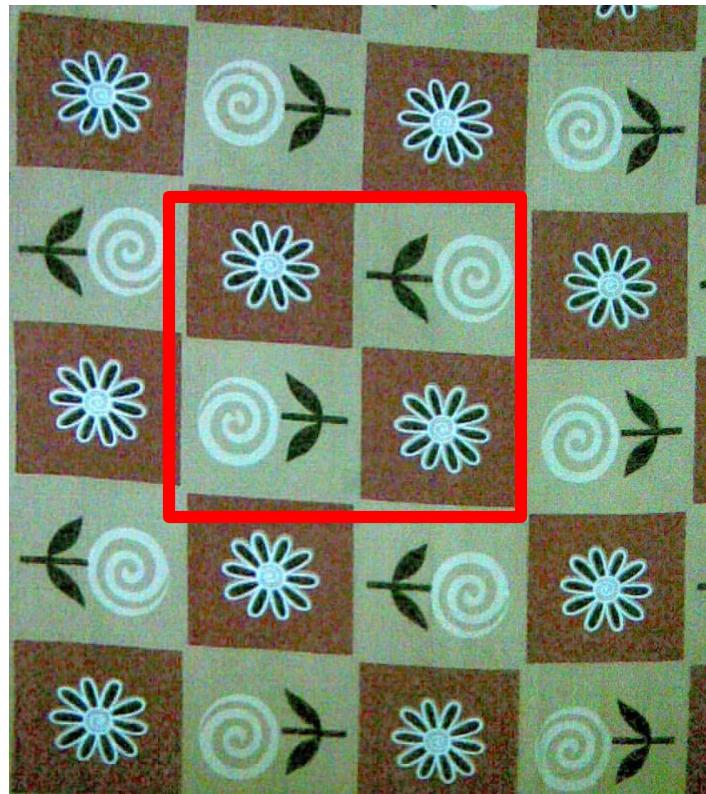
7 Crystal Classes

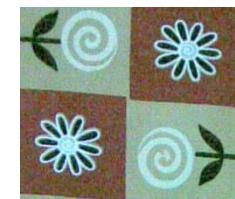
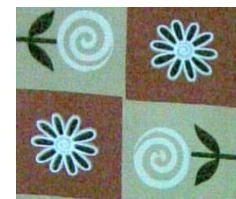
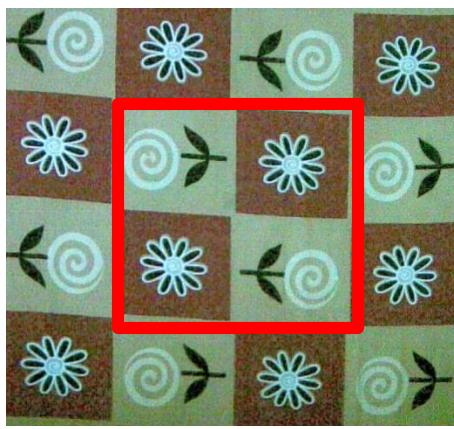
→ 14 Bravais Lattices

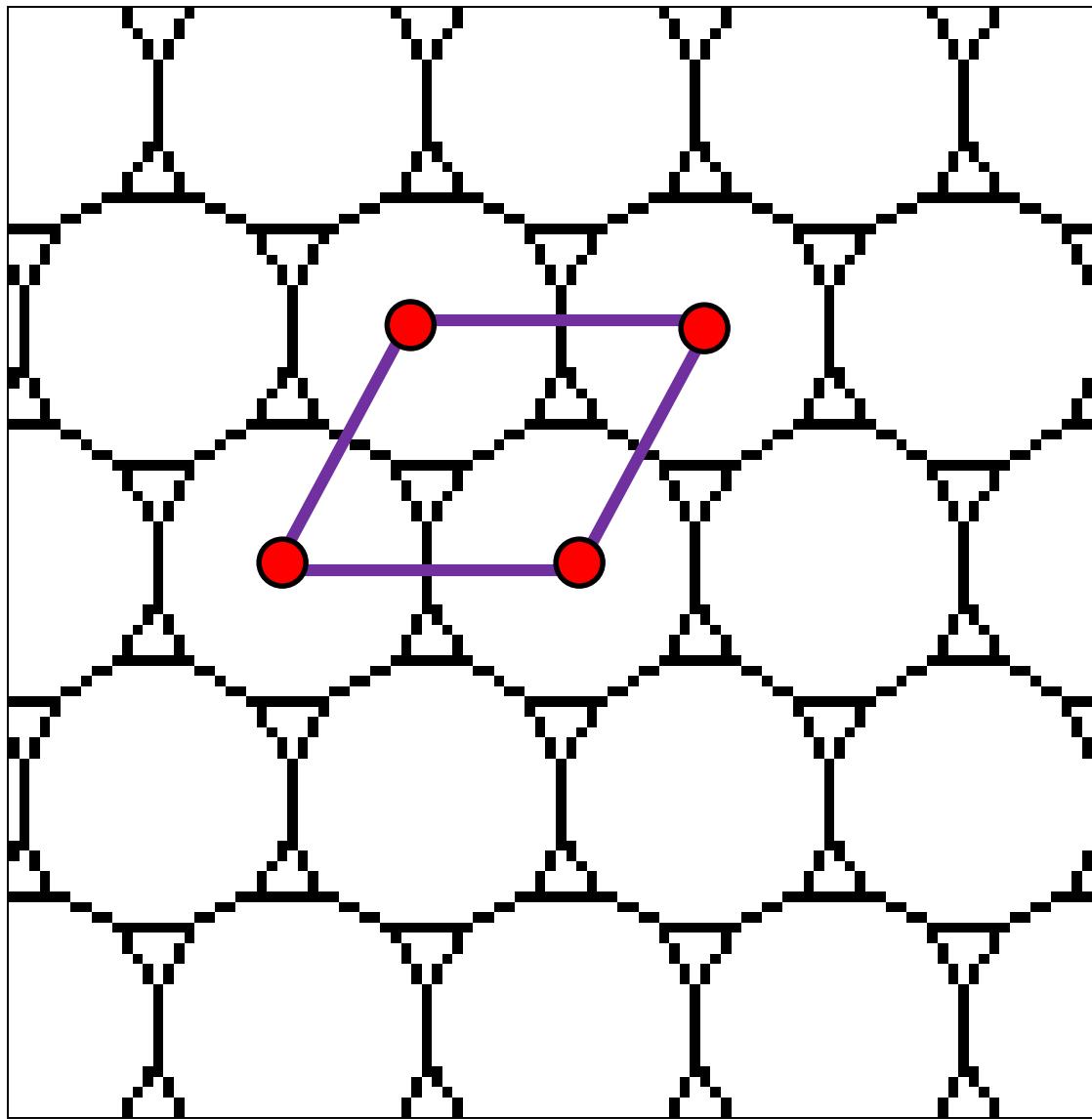
Crystal family	Crystal system	Required symmetries of point group	Point groups	Space groups	Bravais lattices	Lattice system
Triclinic		None	2	2	1	Triclinic
Monoclinic		1 twofold axis of rotation or 1 mirror plane	3	13	2	Monoclinic
Orthorhombic		3 twofold axes of rotation or 1 twofold axis of rotation and two mirror planes.	3	59	4	Orthorhombic
Tetragonal		1 fourfold axis of rotation	7	68	2	Tetragonal
Hexagonal	Trigonal	1 threefold axis of rotation	5	7	1	Rhombohedral
	Hexagonal	1 sixfold axis of rotation	7	18		
Cubic		4 threefold axes of rotation	5	27	1	Hexagonal
Total: 6	7		32	230	14	7

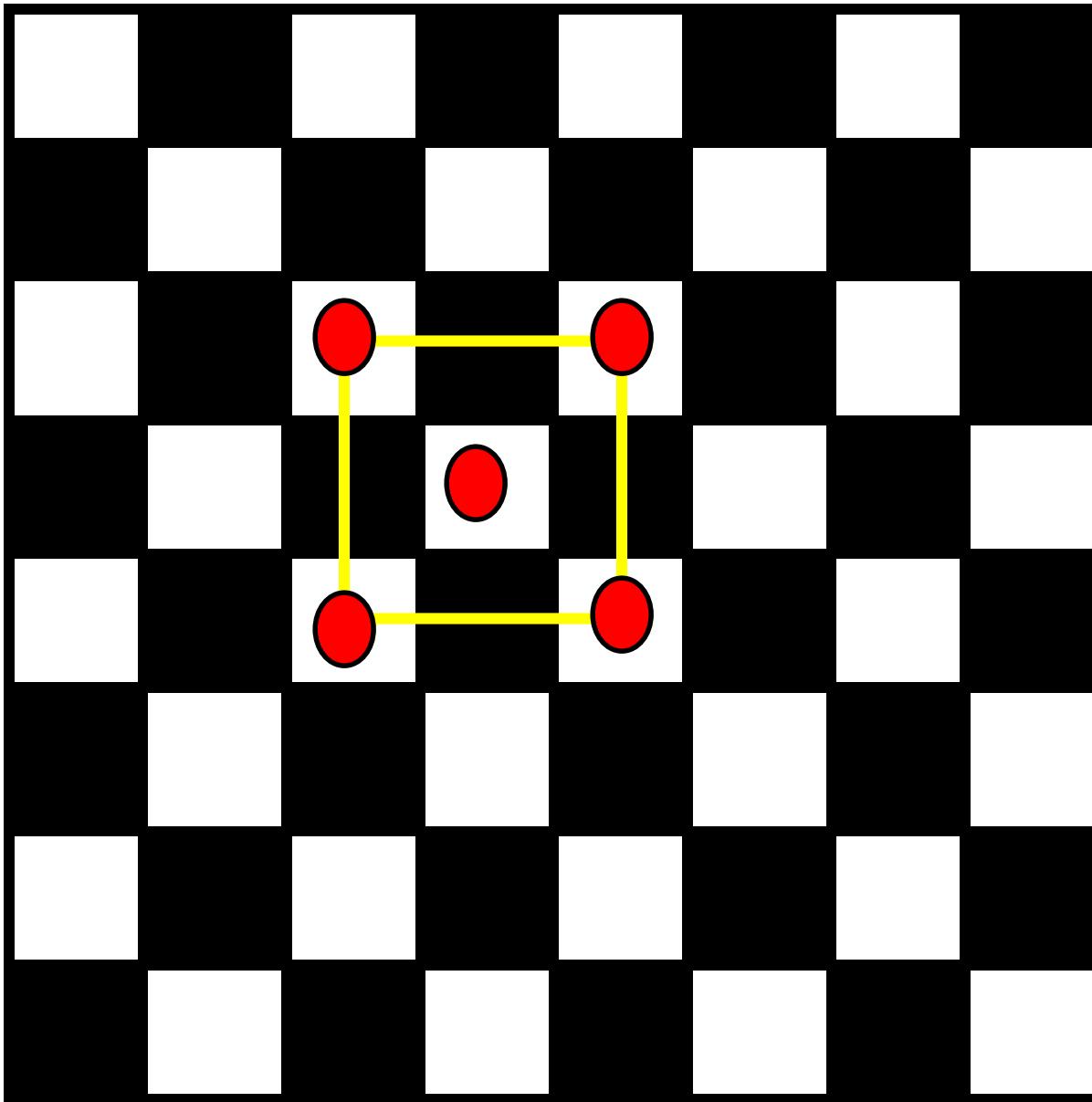


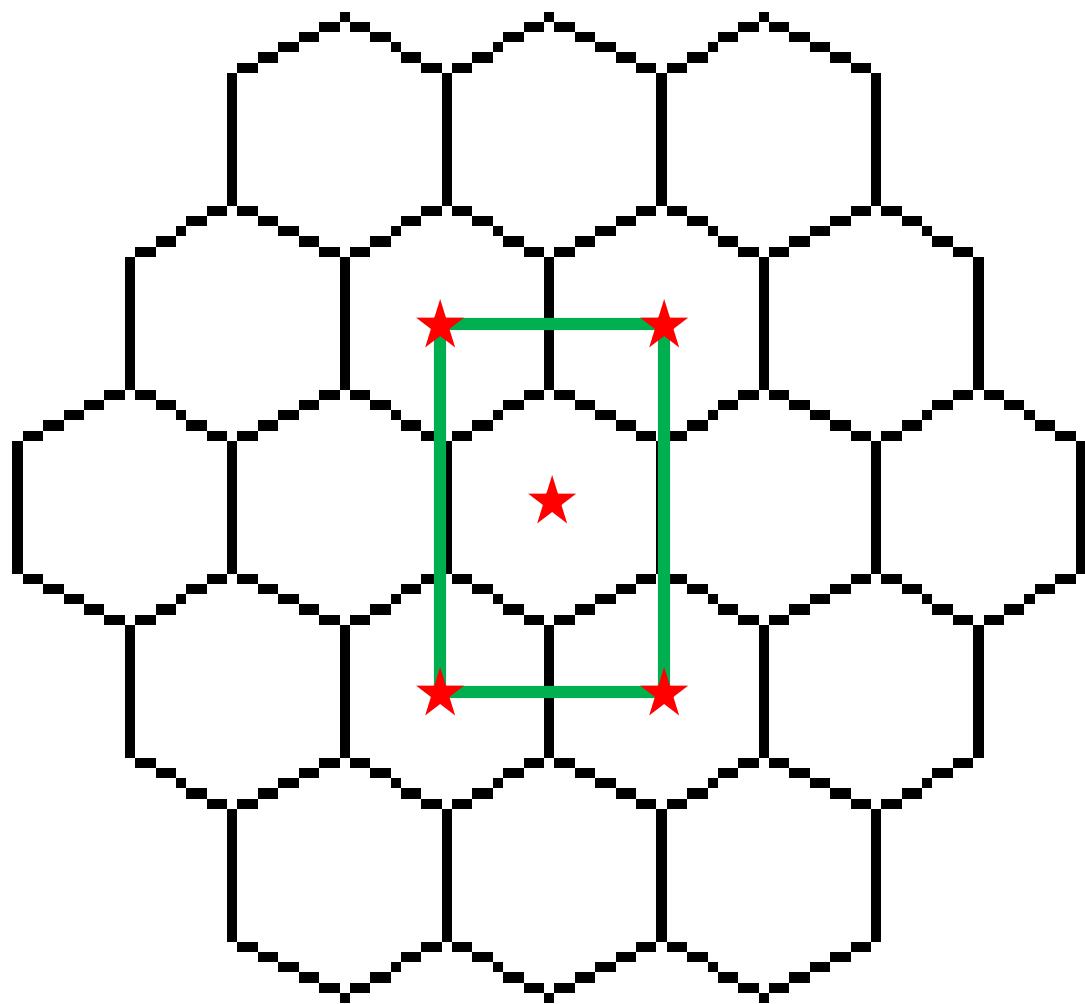


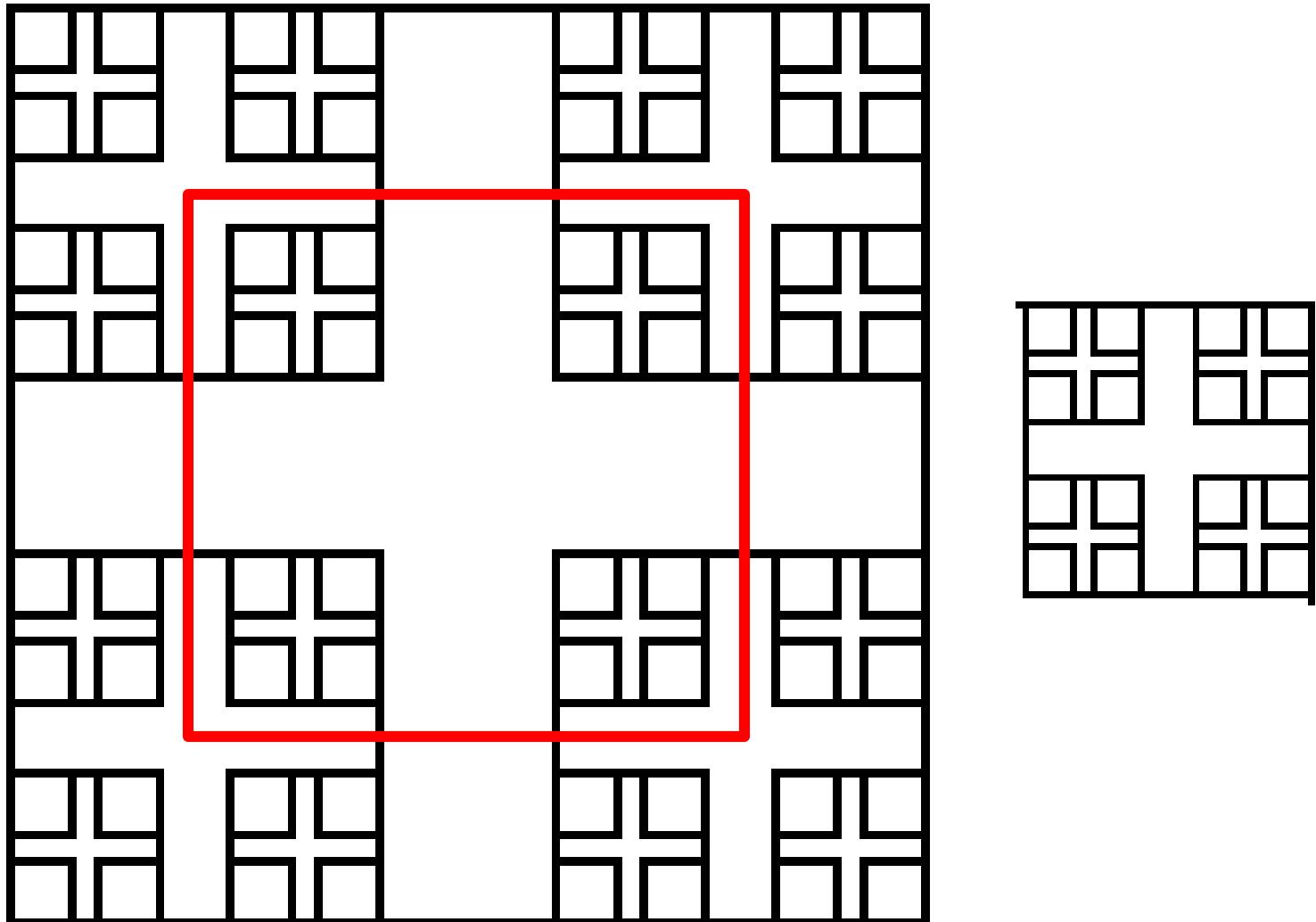




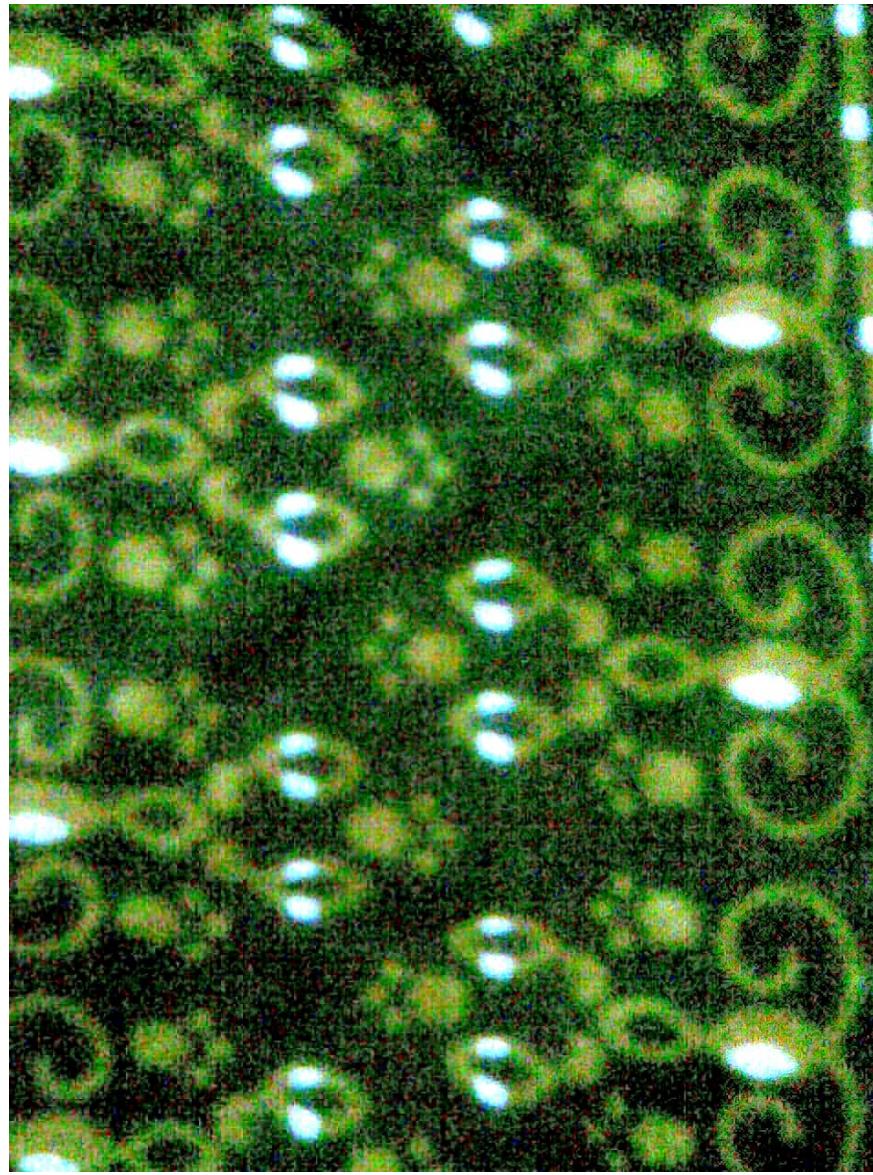


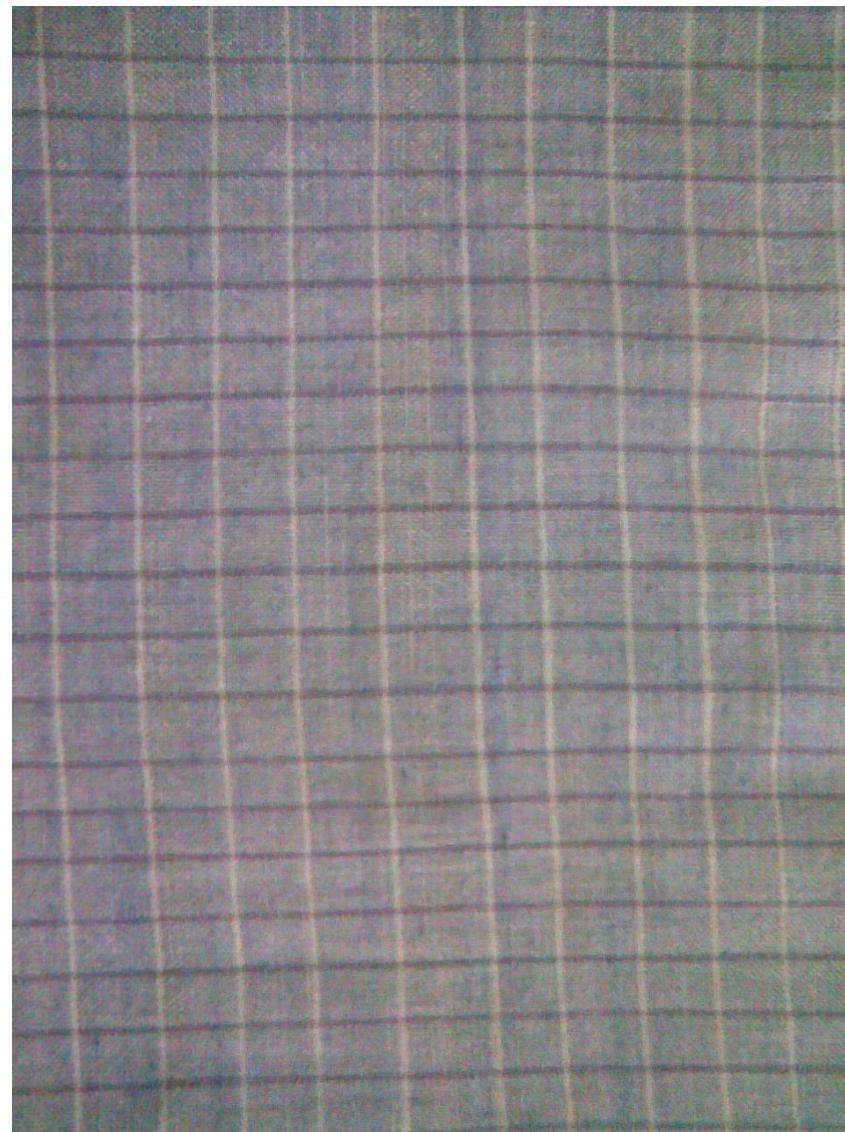














25/01/2009



28/12/2008

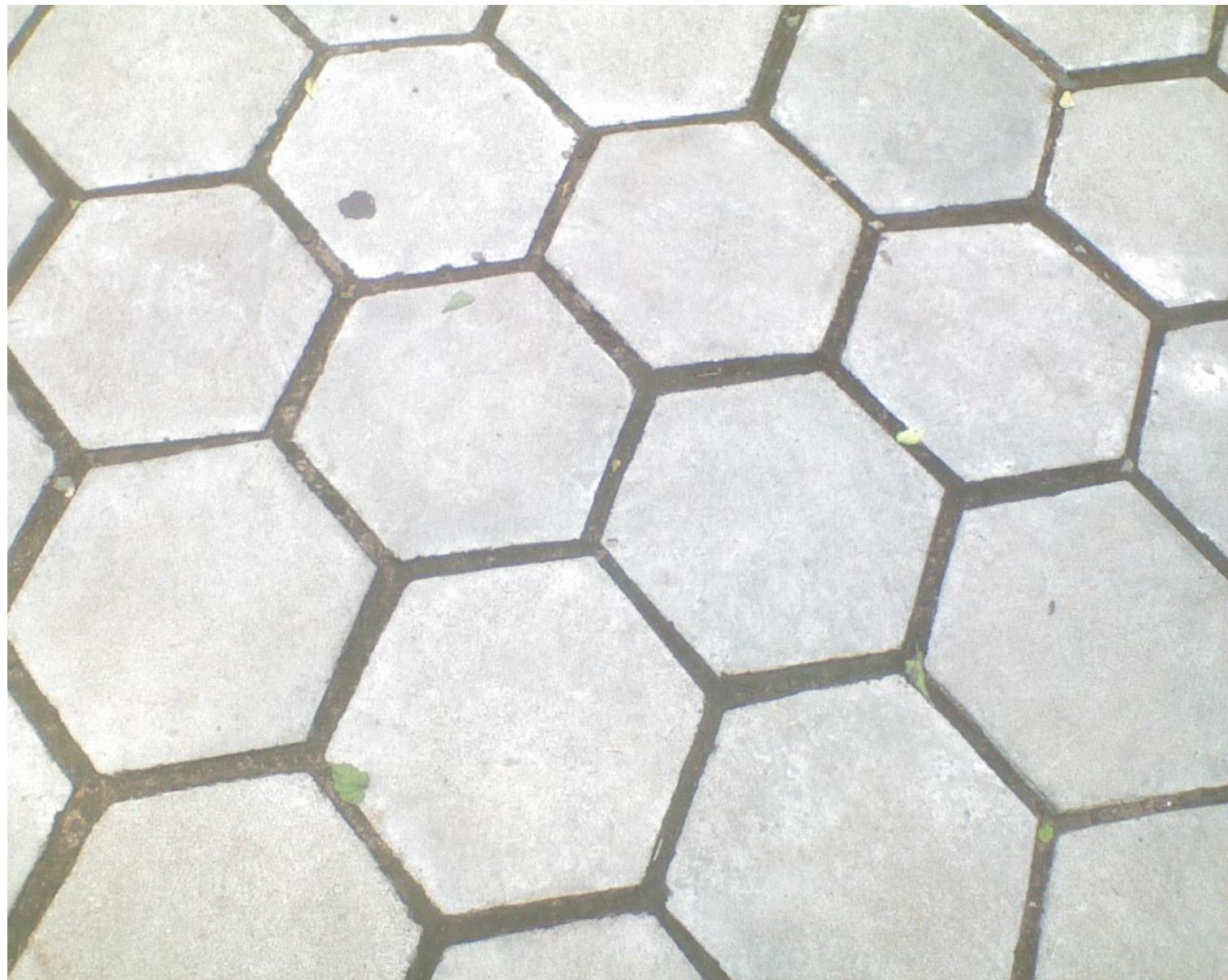


25/01/2009

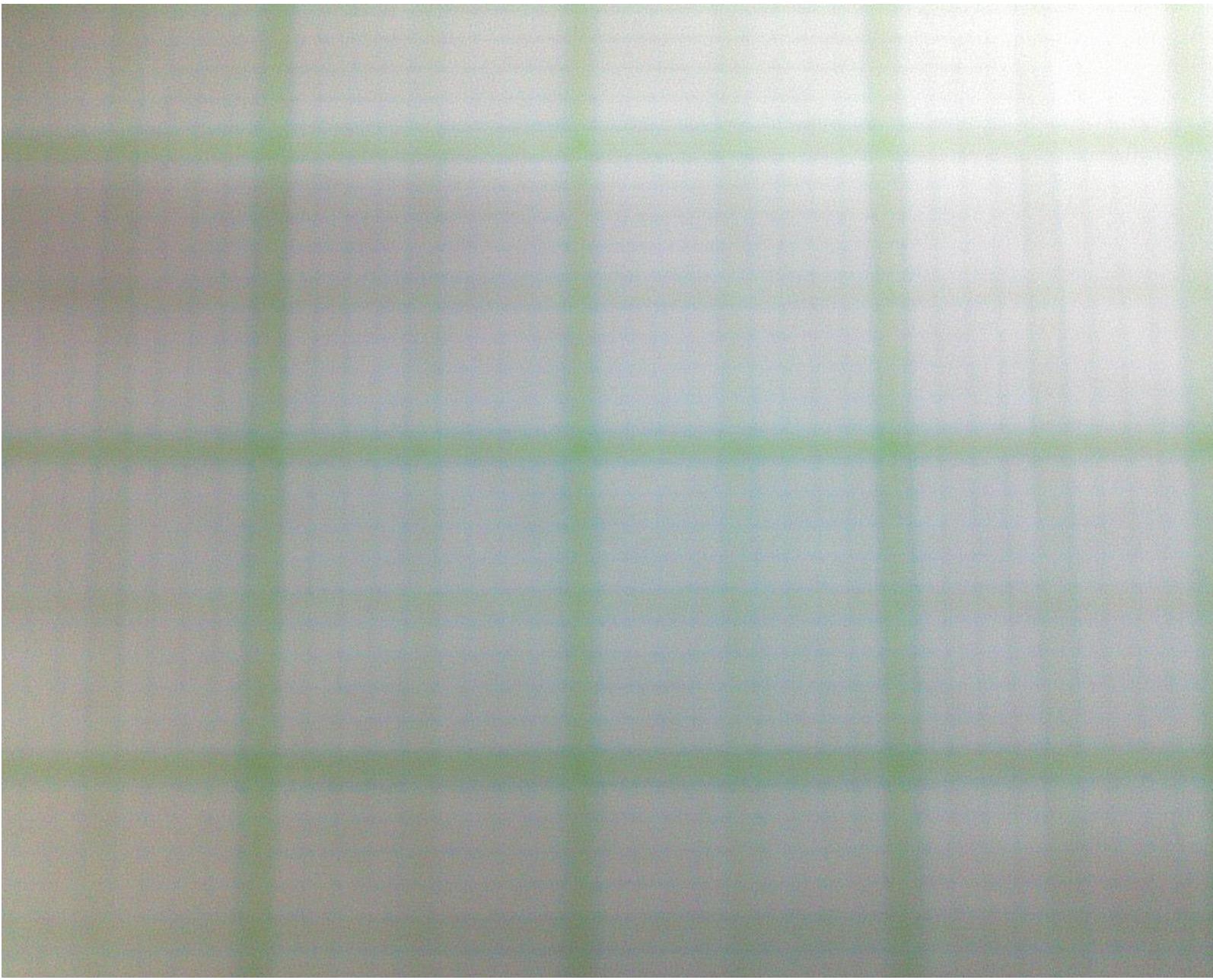


27/01/2009













28/12/2008



28/12/2008



28/12/2008



28/12/2008



28/12/2008



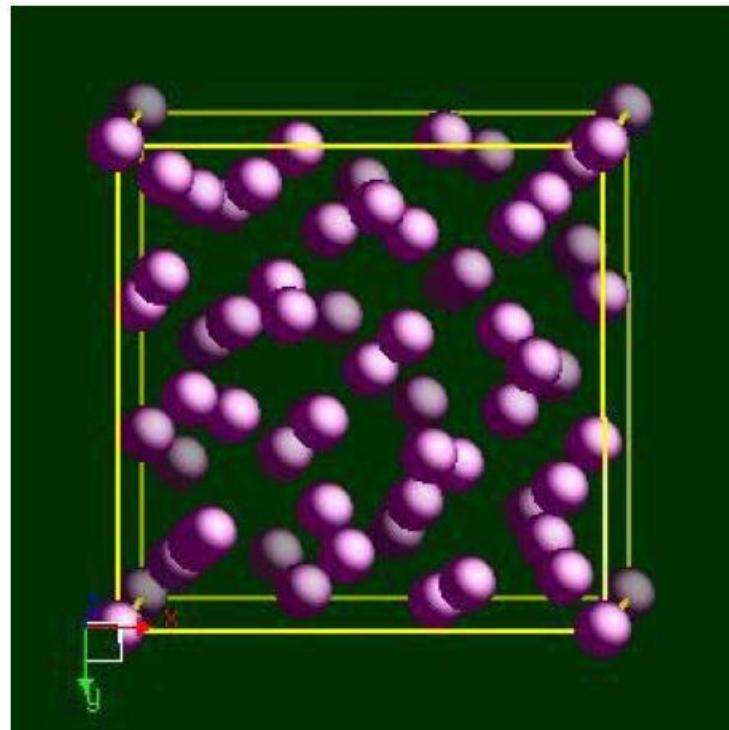
28/12/2008

Manganese: crystal structure

- Space group: I-43m (Space group number: 217)
- Structure: cubic
- Cell parameters:
 - a : 891.25 pm
 - b : 891.25 pm
 - c : 891.25 pm
 - α : 90.000°
 - β : 90.000°
 - γ : 90.000°

Mn

Alpha manganese
58 atoms per unit cell!
Distorted bcc



<http://www.webelements.com/>

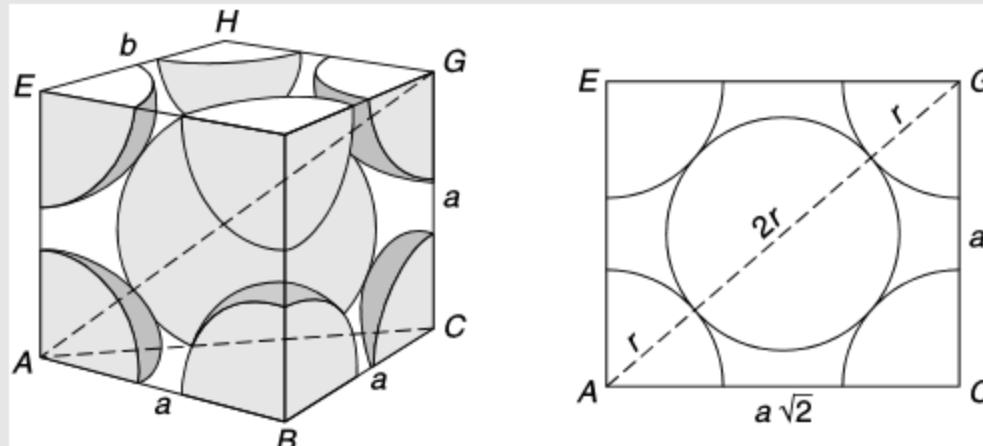
References

C. P. Gazzara, R. M. Middleton, R. J. Weiss, and E. O. Hall, *Acta Crystallogr.*, 1967, **22**, 859.

Example Problem 1.4

Molybdenum has a BCC structure with an atomic radius of 1.36 Å. Calculate the lattice parameter for BCC Mo.

Answer: We know that the molybdenum atoms touch along the body diagonal in BCC, as shown in the projection at right. The length of the body diagonal, then, is $4r$, and is related to the lattice parameter, a (which is the length of the cube edge, not the length of the face diagonal, which is $a\sqrt{2}$) by application of the Pythagorean theorem:



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$$(4r)^2 = a^2 + (a\sqrt{2})^2 = 3a^2$$

$$a = 4r/\sqrt{3} = 4(1.36)/\sqrt{3} = 3.14$$

The lattice parameter for BCC Mo is 3.14 Å, which is consistent with the value in Table 1.11.

Table 1.8 Summary of Important Parameters in the Cubic Space Lattices

	Simple Cubic	Face-Centered Cubic	Body-Centered Cubic
Unit cell side, a	$2r$	$4r/\sqrt{2}$	$4r/\sqrt{3}$
Face diagonal	$\sqrt{2}(2r)$	$4r$	$\sqrt{2/3}(4r)$
Body diagonal	$\sqrt{3}(2r)$	$\sqrt{3/2}(4r)$	$4r$
Number of atoms	1	4	2
Cell volume	$8r^3$	$\frac{32r^3}{\sqrt{2}}$	$\frac{64r^3}{3\sqrt{3}}$

r = atomic radius.

Table 1.12 Some Metal Allotropes

Metal	R.T. Crystal Structure	Structure at Other Temperatures
Ca	FCC	BCC ($>447^{\circ}\text{C}$)
Co	HCP	FCC ($>427^{\circ}\text{C}$)
Hf	HCP	BCC ($>1742^{\circ}\text{C}$)
Fe	BCC	FCC ($>912^{\circ}\text{C}$) BCC ($>1394^{\circ}\text{C}$)
Li	BCC	BCC ($< -193^{\circ}\text{C}$)
Na	BCC	BCC ($< -233^{\circ}\text{C}$)
Sn	BCT	Cubic ($<13^{\circ}\text{C}$)
Tl	HCP	BCC ($>234^{\circ}\text{C}$)
Ti	HCP	BCC ($>883^{\circ}\text{C}$)
Y	HCP	BCC ($>1481^{\circ}\text{C}$)
Zr	HCP	BCC ($>872^{\circ}\text{C}$)

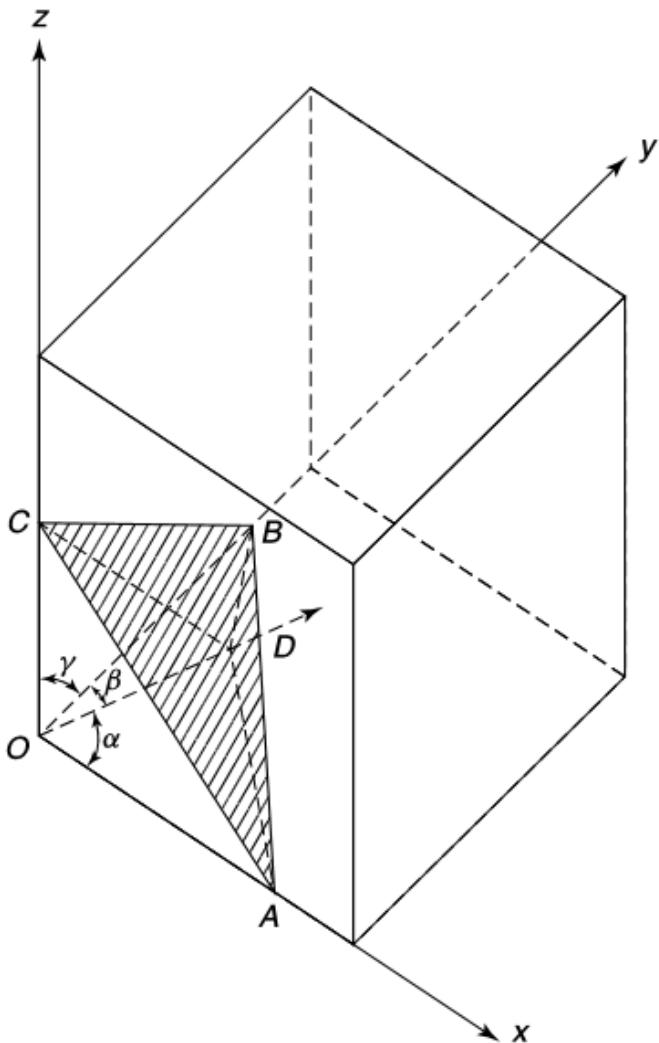


Figure 1.24 Definition of Miller indices for an arbitrary plane (shaded area). From Z. Jastrzebski, *The Nature and Properties of Engineering Materials*, 2nd ed. Copyright @ 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

MILLER INDICES

- PLANES
- DIRECTIONS

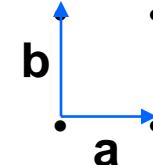
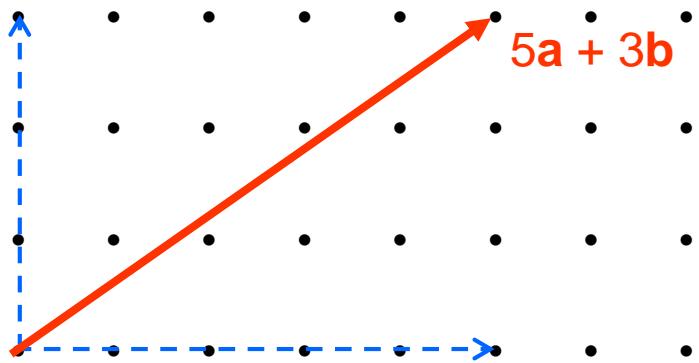
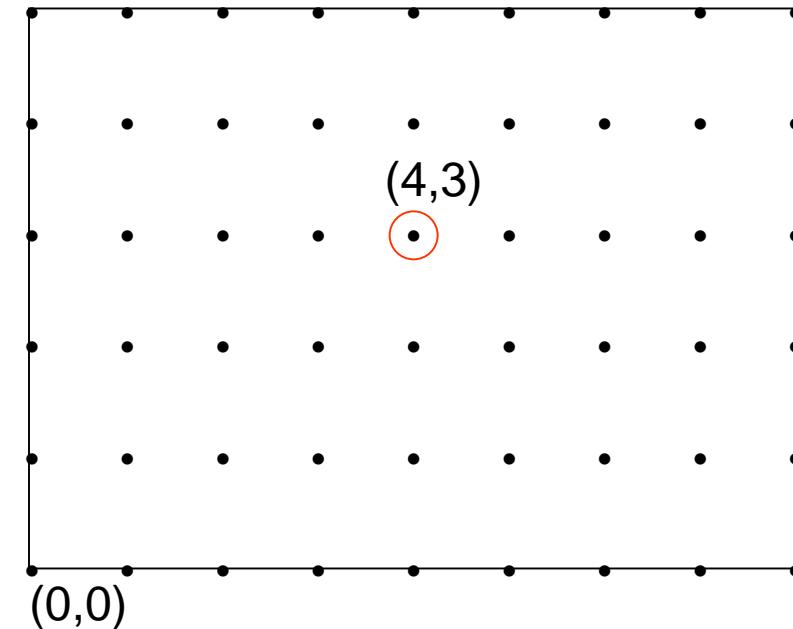
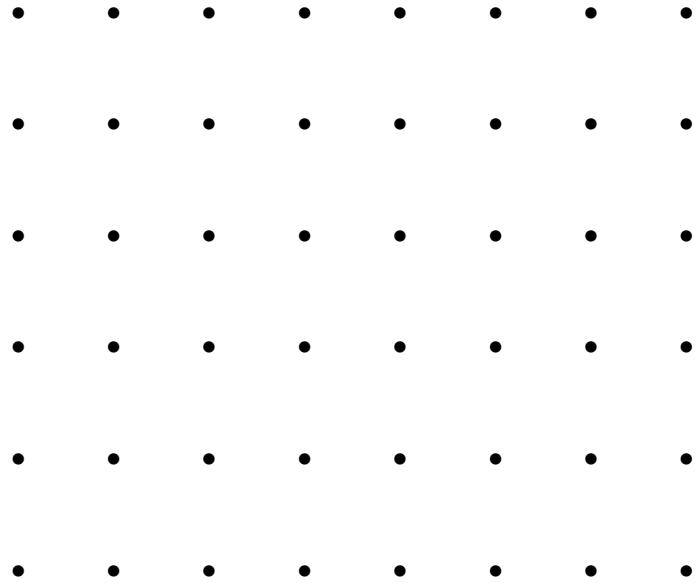
From the law of rational indices developed by French Physicist and mineralogist
Abbé René Just Haüy
and popularized by
William Hallowes Miller

Vector \mathbf{r} passing from the origin to a lattice point:

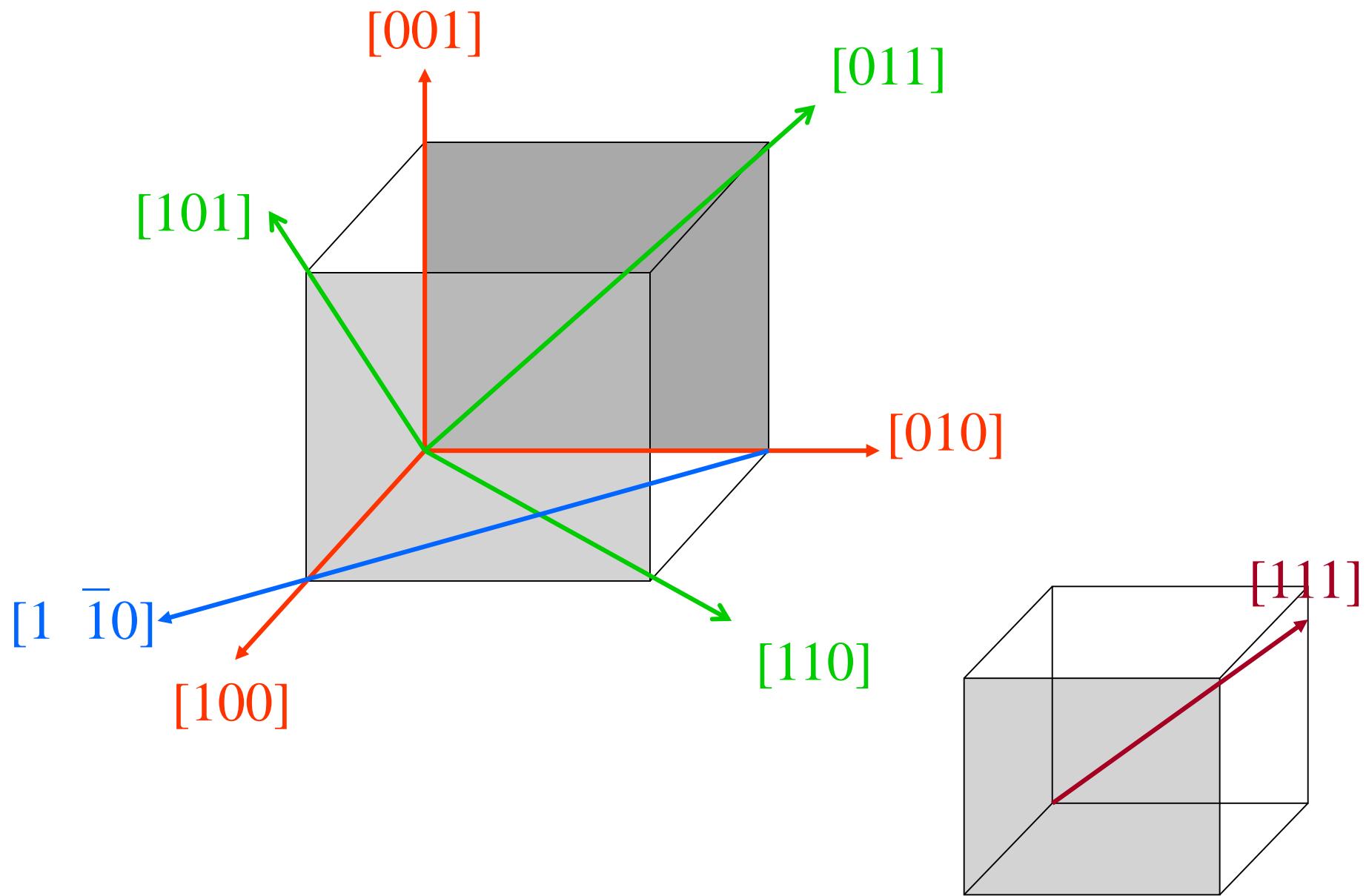
$$\mathbf{r} = r_1 \mathbf{a} + r_2 \mathbf{b} + r_3 \mathbf{c}$$

$\mathbf{a}, \mathbf{b}, \mathbf{c} \rightarrow$ fundamental translation vectors

Miller Indices for directions



Miller indices $\rightarrow [53]$



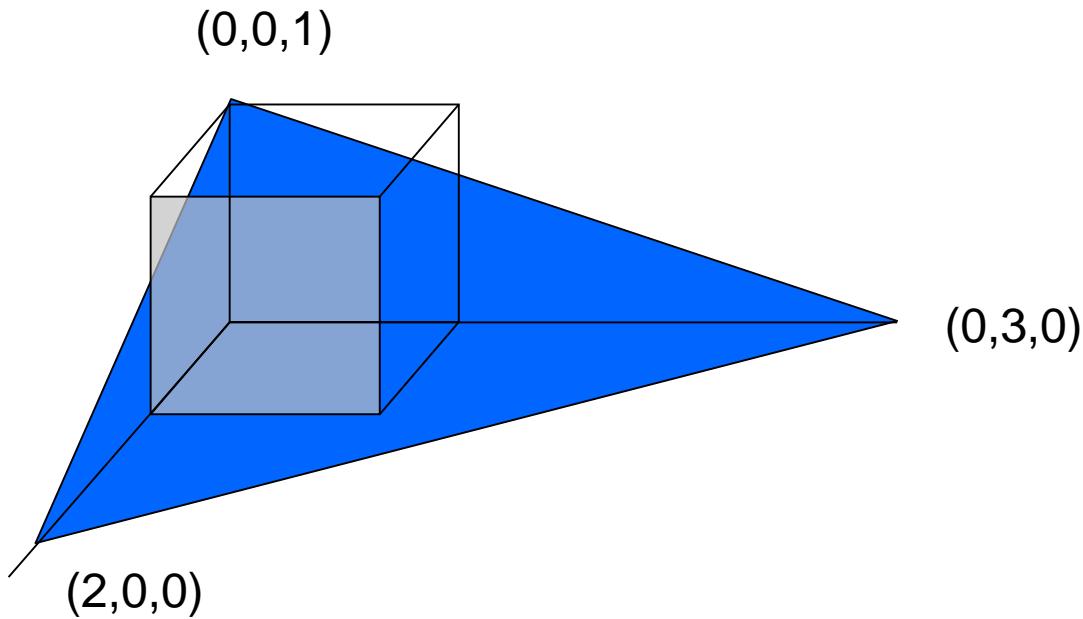
- Coordinates of the final point – coordinates of the initial point
- Reduce to smallest integer values

Family of directions

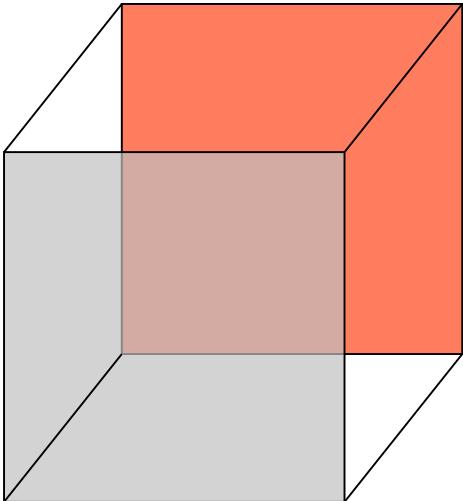
Index		Number in the family for cubic lattice
<100>	→	$3 \times 2 = 6$
<110>	→	$6 \times 2 = 12$
<111>	→	$4 \times 2 = 8$

Symbol	Alternate symbol		
[]		→	Particular direction
< >	[[]]	→	Family of directions

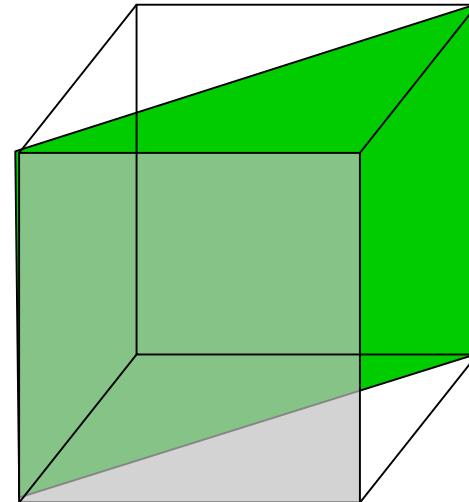
Miller Indices for planes



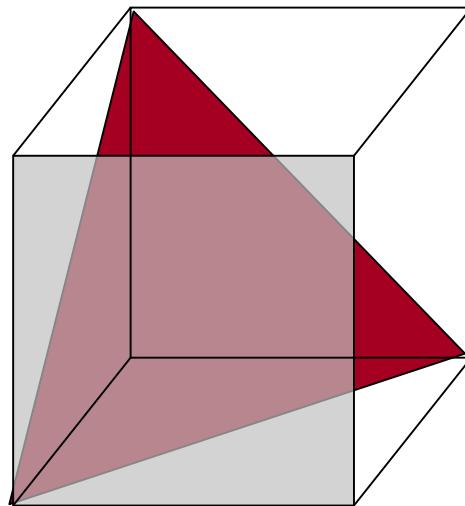
- Find intercepts along axes → 2 3 1
- Take reciprocal → 1/2 1/3 1
- Convert to smallest integers in the same ratio → 3 2 6
- Enclose in parenthesis → (326)



Intercepts $\rightarrow 1 \infty \infty$
Plane $\rightarrow (100)$
Family $\rightarrow \{100\} \rightarrow 3$



Intercepts $\rightarrow 1 1 \infty$
Plane $\rightarrow (110)$
Family $\rightarrow \{110\} \rightarrow 6$



Intercepts $\rightarrow 1 1 1$
Plane $\rightarrow (111)$
Family $\rightarrow \{111\} \rightarrow 8$
(Octahedral plane)

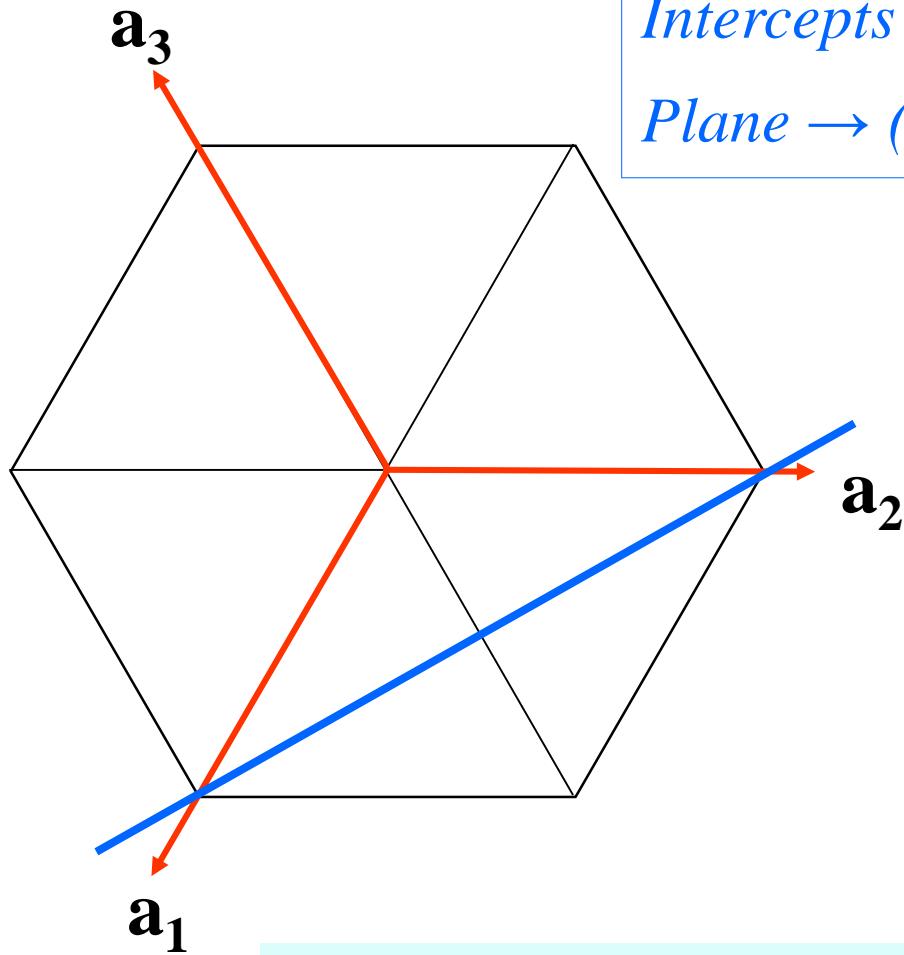
Summary of notations

	Symbol		Alternate symbols		
Direction	[]	[uvw]		→	Particular direction
	< >	<uvw>	[[]]	→	Family of directions
Plane	()	(hkl)		→	Particular plane
	{ }	{hkl}	(())	→	Family of planes
Point	..	.xyz.	[[]]	→	Particular point
	::	:xyz:		→	Family of point

A family is also referred to as a *symmetrical set*

- Unknown direction → [uvw]
- Unknown plane → (hkl)
- Double digit indices should be separated by commas → (12,22,3)
- In cubic crystals $[hkl] \perp (hkl)$

Hexagonal crystals → Miller-Bravais Indices

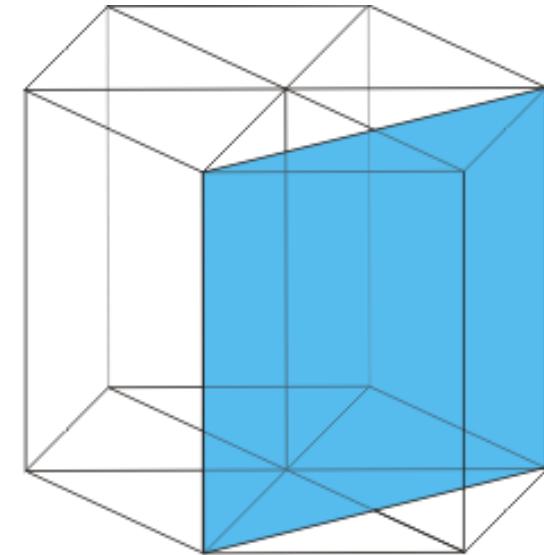


Intercepts → 1 1 - 1/2 ∞

Plane → (1 1 2̄ 0)

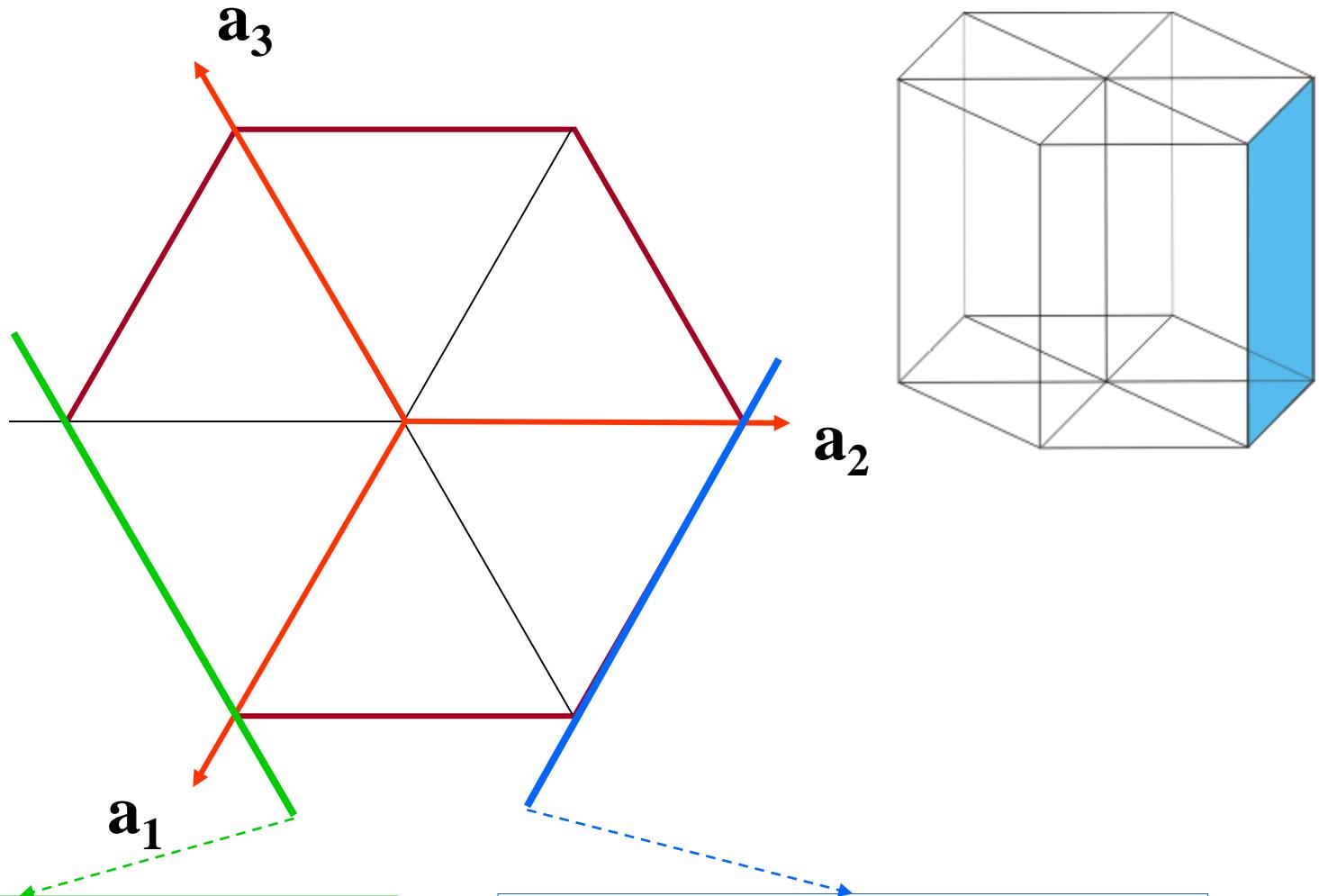
($h k i l$)

$$i = -(h + k)$$



The use of the 4 index notation is to bring out the equivalence between crystallographically equivalent planes and directions

Examples to show the utility of the 4 index notation



Intercepts $\rightarrow 1 -1 \infty \infty$

Miller $\rightarrow (1 \bar{1} 0)$

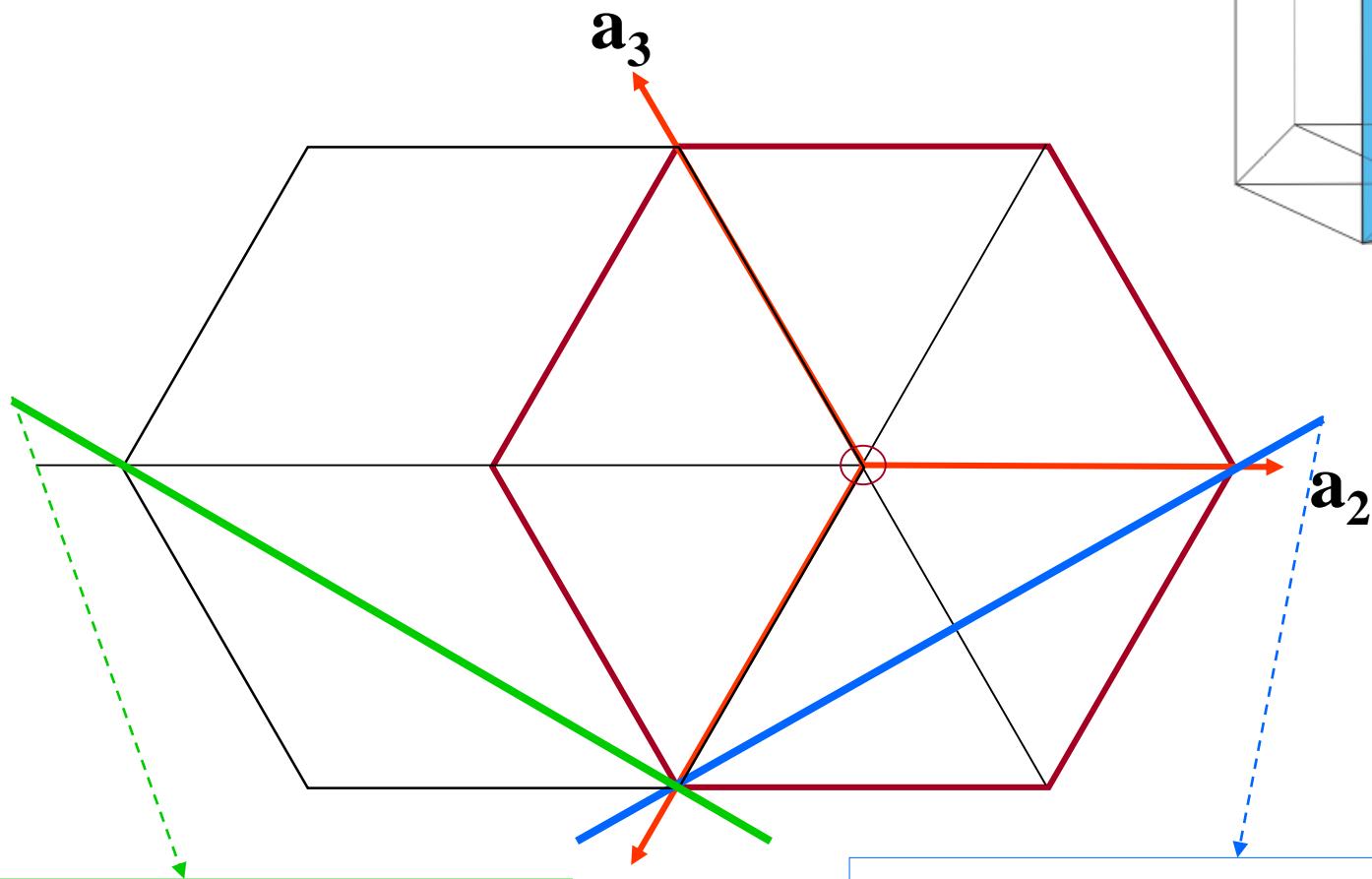
Miller-Bravais $\rightarrow (1 \bar{1} 0 0)$

Intercepts $\rightarrow \infty 1 -1 \infty$

Miller $\rightarrow (0 1 0)$

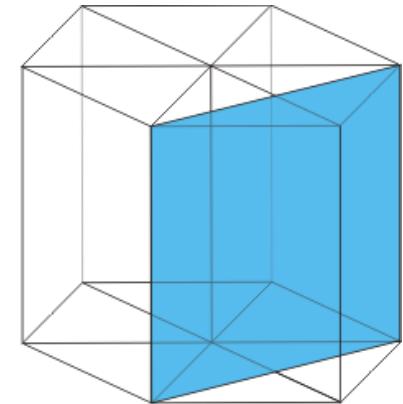
Miller-Bravais $\rightarrow (0 1 \bar{1} 0)$

Examples to show the utility of the 4 index notation



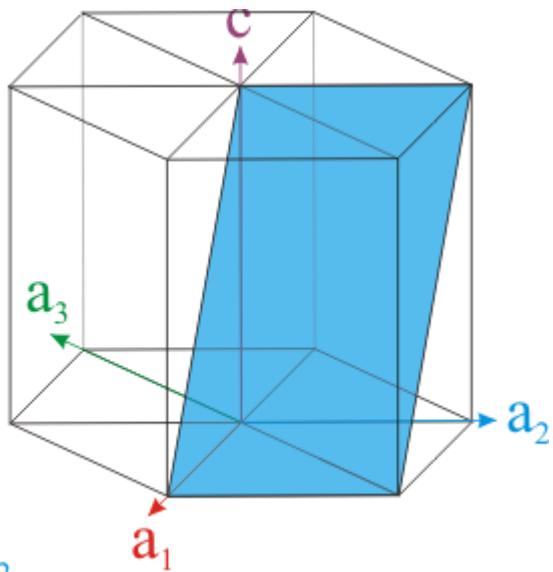
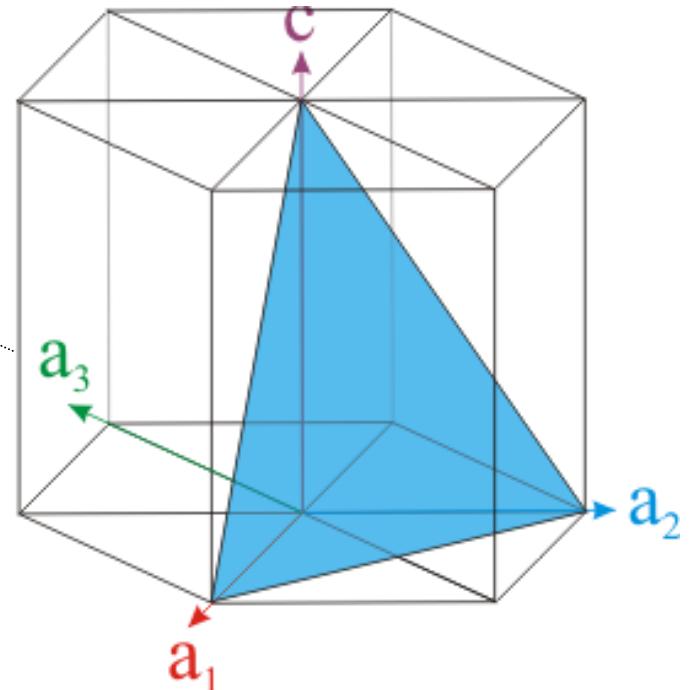
Intercepts $\rightarrow 1 \ -2 \ -2 \ \infty$
Plane $\rightarrow (2 \ -1 \ 1 \ 0)$

Intercepts $\rightarrow 1 \ 1 \ -\frac{1}{2} \ \infty$
Plane $\rightarrow (1 \ 1 \ \bar{2} \ 0)$



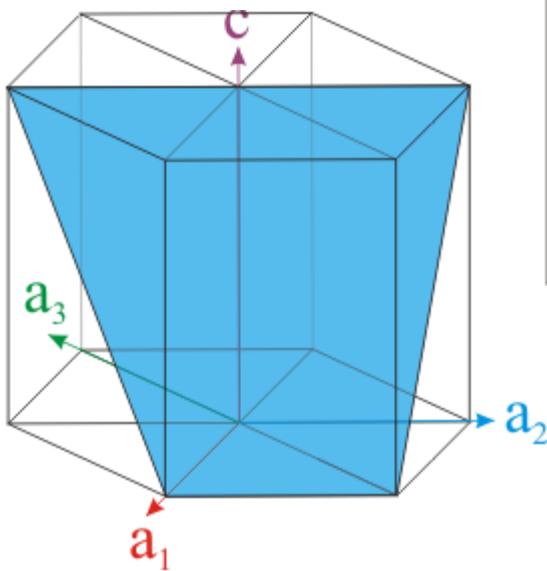
Intercepts $\rightarrow 1 \ 1 - \frac{1}{2} \ 1$

Plane $\rightarrow (1 \ 1 \ \bar{2} \ 1)$



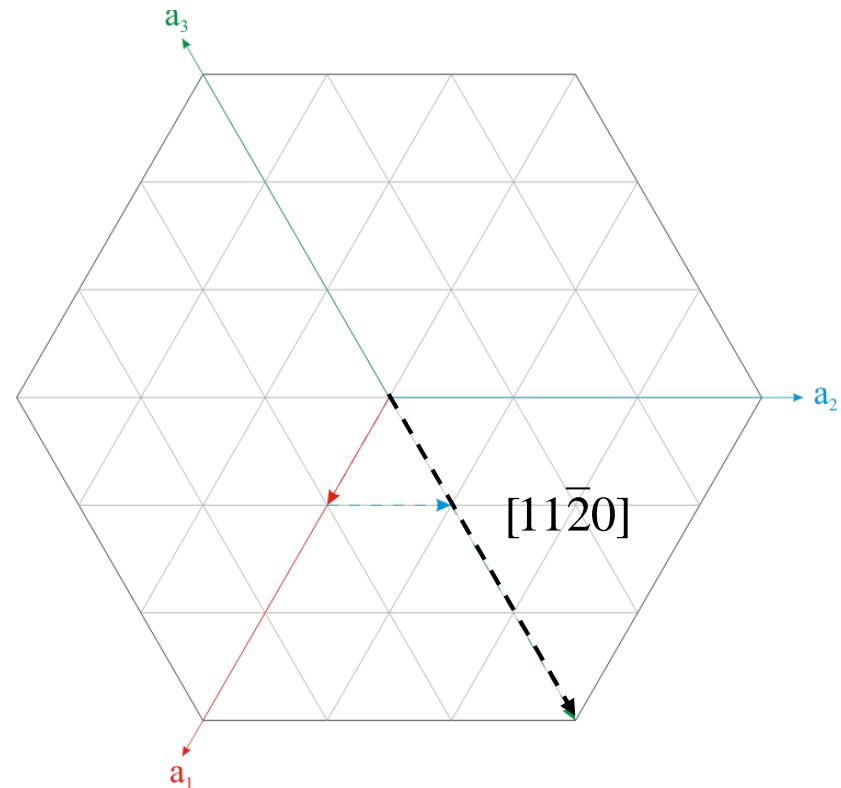
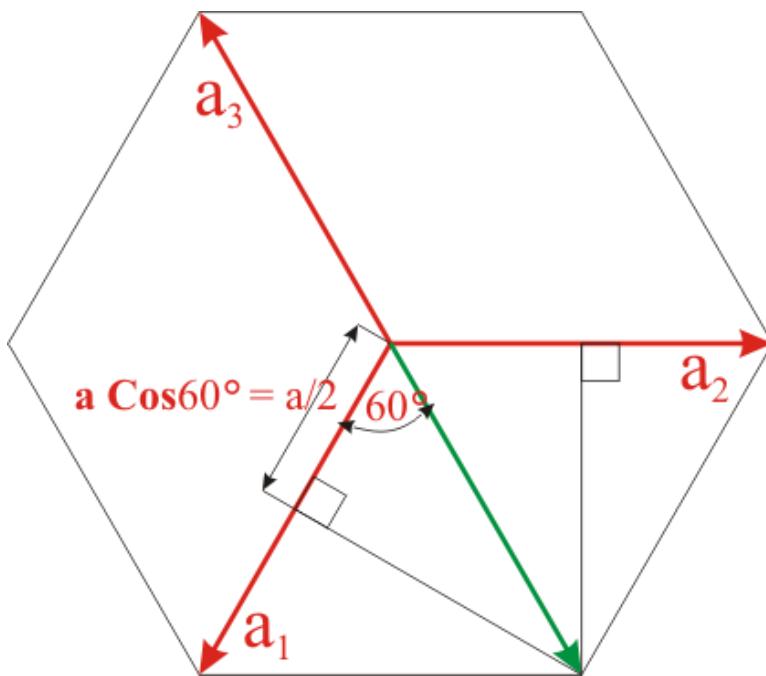
Intercepts $\rightarrow 1 \ \infty - 1 \ 1$

Plane $\rightarrow (1 \ 0 \ \bar{1} \ 1)$

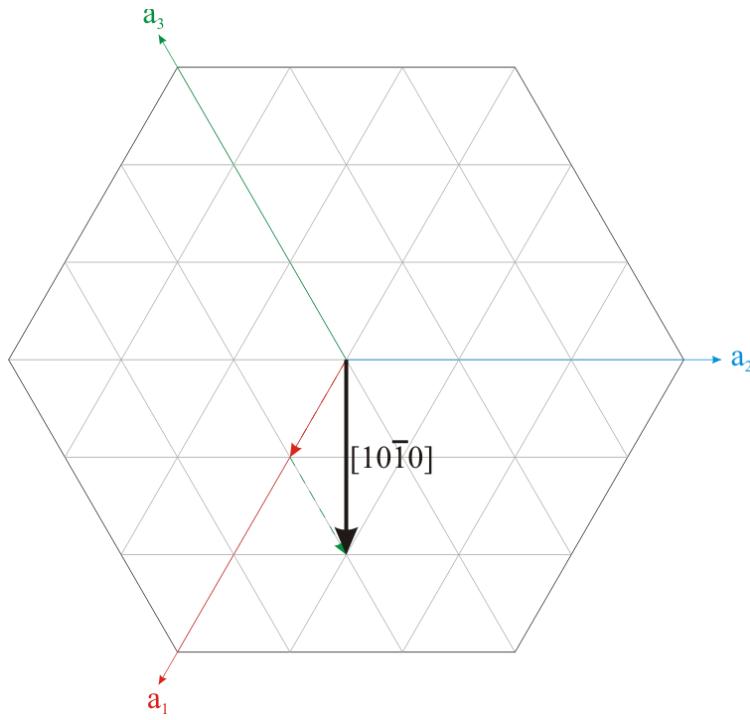


Directions

Directions are projected onto the basis vectors to determine the components



	a_1	a_2	a_3
Projections	$a/2$	$a/2$	$-a$
Normalized wrt LP	$1/2$	$1/2$	-1
Factorization	1	1	-2
Indices	$[1 \ 1 \ \bar{2} \ 0]$		



Transformation between 3-index $[UVW]$ and 4-index $[uvtw]$ notations

$$U = u - t$$

$$V = v - t$$

$$W = w$$

$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2V - U)$$

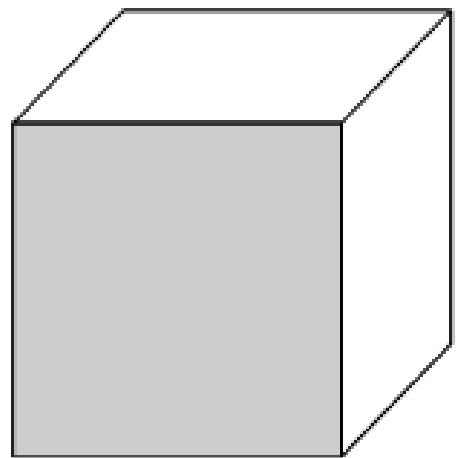
$$t = -(u + v)$$

$$w = W$$

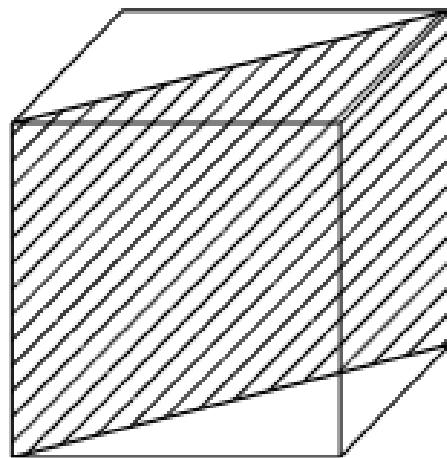
- Directions in the hexagonal system can be expressed in many ways
- 3-indices:
By the three vector components along a_1 , a_2 and c :
 $r_{UVW} = Ua_1 + Va_2 + Wc$
- In the three index notation equivalent directions may not seem equivalent
- 4-indices:

Directions \perp Planes

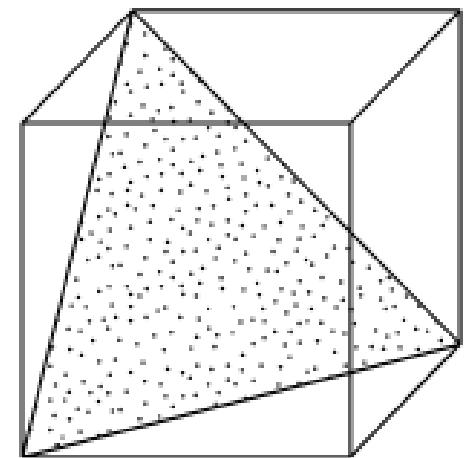
- Cubic system:** $(hkl) \perp [hkl]$
- Tetragonal system:** only special planes are \perp to the direction with same indices:
 $[100] \perp (100)$, $[010] \perp (010)$, $[001] \perp (001)$, $[110] \perp (110)$
 $([101] \text{ not } \perp (101))$
- Orthorhombic system:**
 $[100] \perp (100)$, $[010] \perp (010)$, $[001] \perp (001)$
- Hexagonal system:** $[0001] \perp (0001)$
(this is for a general c/a ratio; for a Hexagonal crystal with the special c/a ratio = $\sqrt{3}/2$ the cubic rule is followed)
- Monoclinic system:** $[010] \perp (010)$
- Other than these a general $[hkl]$ is NOT $\perp (hkl)$



(100)



(110)



(111)

Figure 1.25 Some important planes in the cubic space lattice.

$$d = V \left[\begin{array}{l} h^2 b^2 c^2 \sin^2 \alpha + k^2 a^2 c^2 \sin^2 \beta + l^2 a^2 b^2 \sin^2 \gamma \\ + 2hla b^2 c (\cos \alpha \cos \gamma - \cos \beta) + 2hkabc^2 (\cos \alpha \cos \beta - \cos \gamma) \\ + 2kla^2 bc (\cos \beta \cos \gamma - \cos \alpha) \end{array} \right]^{-1/2}$$

$$\frac{1}{d} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right)^{1/2}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Index	Number of members in a cubic lattice	d_{hkl}	
(100)	6	$d_{100} = a$	
(110)	12	$d_{100} = a/\sqrt{2} = a\sqrt{2}/2$	The (110) plane bisects the face diagonal
(111)	8	$d_{100} = a/\sqrt{3} = a\sqrt{3}/3$	The (111) plane trisects the body diagonal
(210)	24		
(211)	24		
(221)	24		
(310)	24		
(311)	24		
(320)	24		
(321)	48		

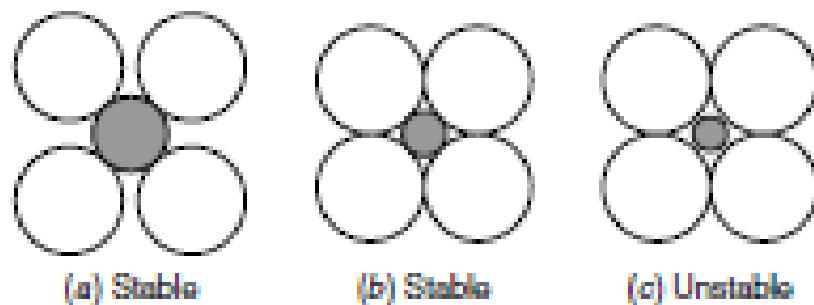


Figure 1.36 (a, b) Stable and (c) unstable coordination configurations. From W. D. Kingery, H. K. Bowen, and D. R. Uhlmann, *Introduction to Ceramics*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

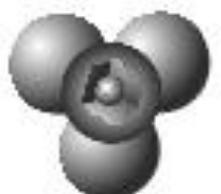
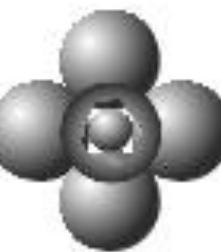
Coordination Number	Anion-Cation Radius Ratio	Coordination Geometry
2	> 6.45	
3	4.45-6.45	
4	2.42-4.45	
6	1.37-2.42	
8	1.0-1.37	

Figure 1.37 Critical radius ratios for various coordination numbers. Adapted, from W. Callister, *Materials Science and Engineering: An Introduction*, 5th ed., p. 384. Copyright © 2000 by John Wiley & Sons, Inc.

PAULING'S RULES

1. *Coordination polyhedra are formed. Radius Ratio is important in determining stability.*
2. Local electrical neutrality is maintained.
3. Corners, rather than faces or edges, tend to be shared in stable structures.
4. Pauling's fourth rule is similar to the third, stating that polyhedra formed about cations of low coordination number and high charge tend to be linked by corners.
5. The number of different constituents in a structure tends to be small

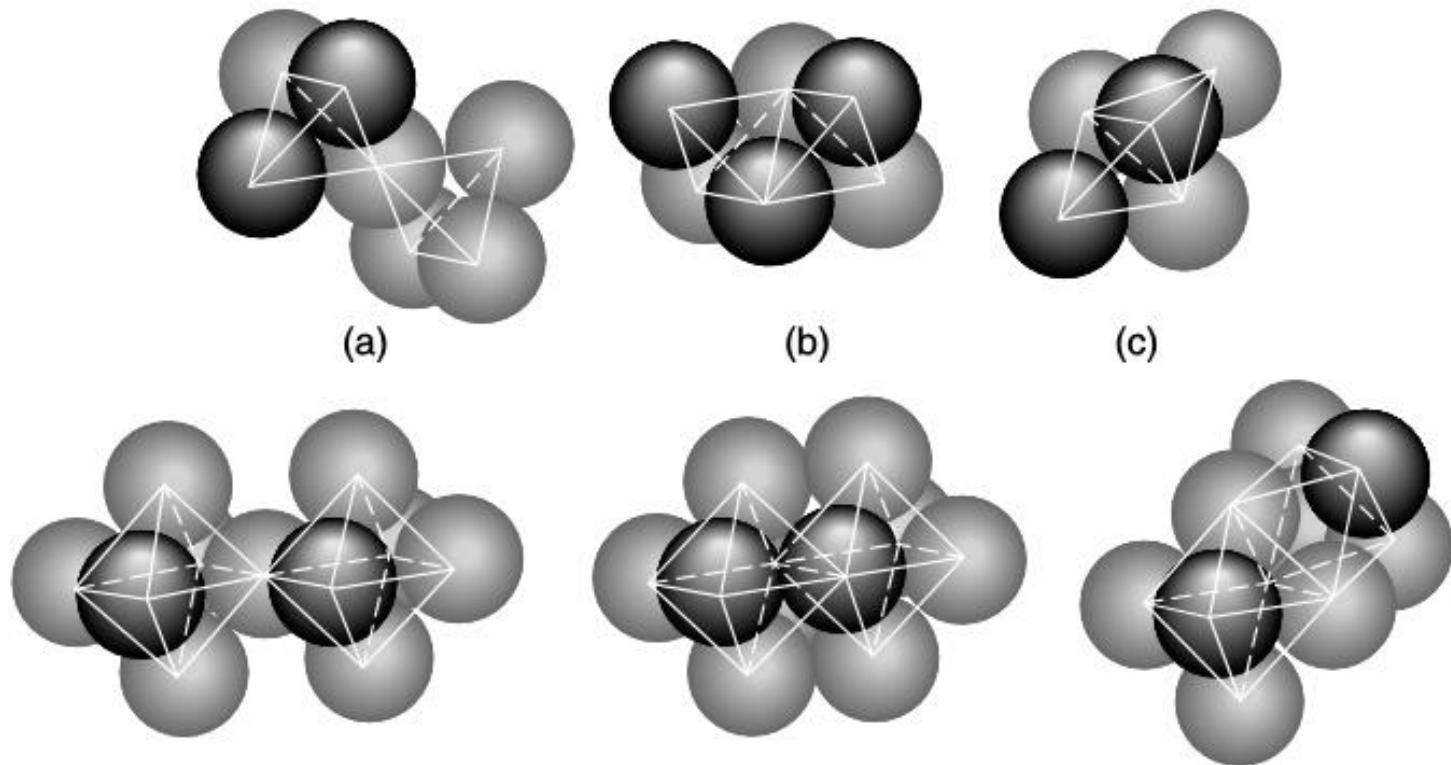


Figure 1.38 Tetrahedra (*top*) and octahedra (*bottom*) linked by sharing (a) corners, (b) edges, and (c) faces. From W. D. Kingery, H. K. Bowen, and D. R. Uhlmann, *Introduction to Ceramics*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

Table 1.16 Table of Some Simple Ionic Structures and Their Corresponding Coordination Numbers

Anion Packing	Coordination Number of M and O	Sites by Cations	Structure Name	Examples
Cubic close-packed	6:6 MO	All oct.	Rock salt	NaCl, KCl, LiF, KBr, MgO, CaO, SrO, BaO, CdO, VO, MnO, FeO, CoO, NiO
Cubic close-packed	4:4 MO	1/2 tet.	Zinc blende	ZnS, BeO, SiC
Cubic close-packed	4:8 M ₂ O	All tet.	Antifluorite	Li ₂ O, Na ₂ O, K ₂ O, Rb ₂ O, sulfides
Distorted cubic close-packed	6:3 MO ₂	1/2 oct.	Rutile	TiO ₂ , GeO ₂ , SnO ₂ , PbO ₂ , VO ₂ , NbO ₂ , TeO ₂ , MnO ₂ , RuO ₂ , OsO ₂ , IrO ₂
Cubic close-packed	12:6:6 ABO ₃	1/4 oct. (B)	Perovskite	CoTiO ₃ , SrTiO ₃ , SrSnO ₃ , SrZrO ₃ , SrHfO ₃ , BaTiO ₃
Cubic close-packed	4:6:4 AB ₂ O ₄	1/8 tet. (A) 1/2 oct. (B)	Spinel	FeAl ₂ O ₄ , ZnAl ₂ O ₄ , MgAl ₂ O ₄
Cubic close-packed	4:6:4 B(AB)O ₄	1/8 tet. (B) 1/2 oct. (A, B)	Spinel (inverse)	FeMgFeO ₄ , MgTiMgO ₄
Hexagonal close-packed	4:4 MO	1/2 tet.	Wurtzite	ZnS, ZnO, SiC
Hexagonal close-packed	6:6 MO	All oct.	Nickel arsenide	NiAs, FeS, FeSe, CoSe
Hexagonal close-packed	6:4 M ₂ O ₃	2/3 oct.	Corundum	Al ₂ O ₃ , Fe ₂ O ₃ , Cr ₂ O ₃ , Ti ₂ O ₃ , V ₂ O ₃ , Ga ₂ O ₃ , Rh ₂ O ₃
Hexagonal close-packed	6:6:4 ABO ₃	2/3 oct. (A, B)	Ilmenite	FeTiO ₃ , NiTiO ₃ , CoTiO ₃
Hexagonal close-packed	6:4:4 A ₂ BO ₄	1/2 oct. (A) 1/8 tet. (B)	Olivine	Mg ₂ SiO ₄ , Fe ₂ SiO ₄
Simple cubic	8:8 MO	All cubic	CsCl	CsCl, CsBr, CsI
Simple cubic	8:4 MO ₂	1/2 cubic	Fluorite	ThO ₂ , CeO ₂ , PrO ₂ , UO ₂ , ZrO ₂ , HfO ₂ , NpO ₂ , PuO ₂ , AmO ₂
Connected tetrahedra	4:2 MO ₂	—	Silica types	SiO ₂ , GeO ₂

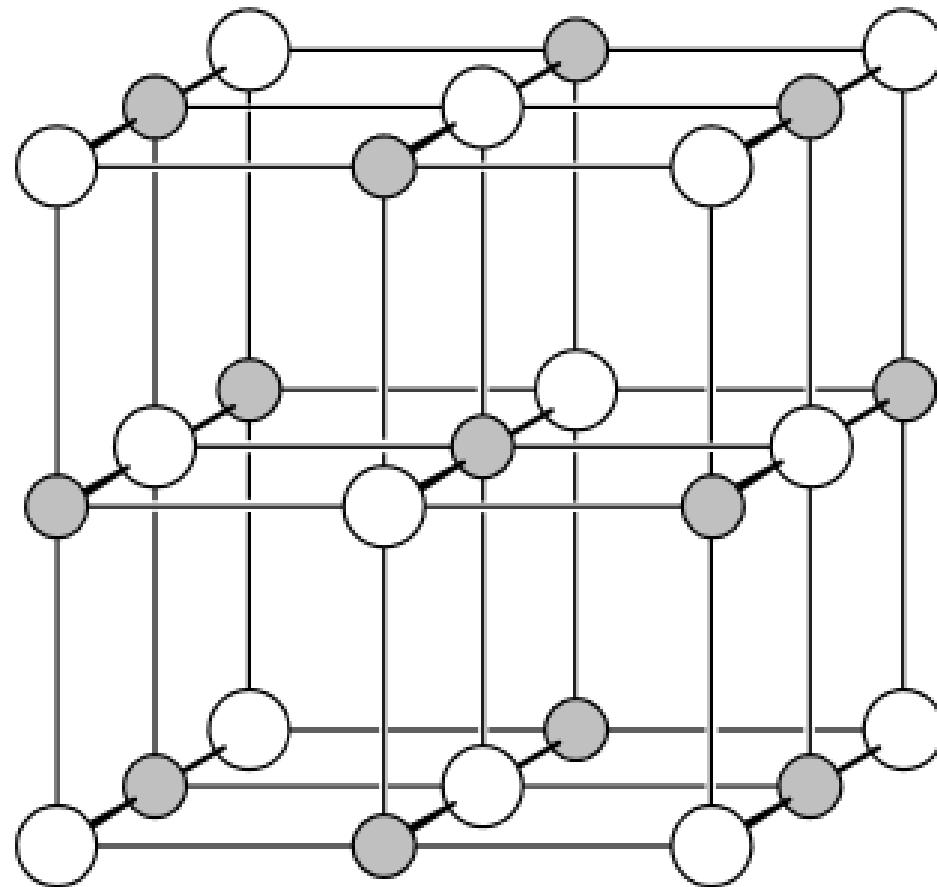


Figure 1.39 The rock salt crystal structure.

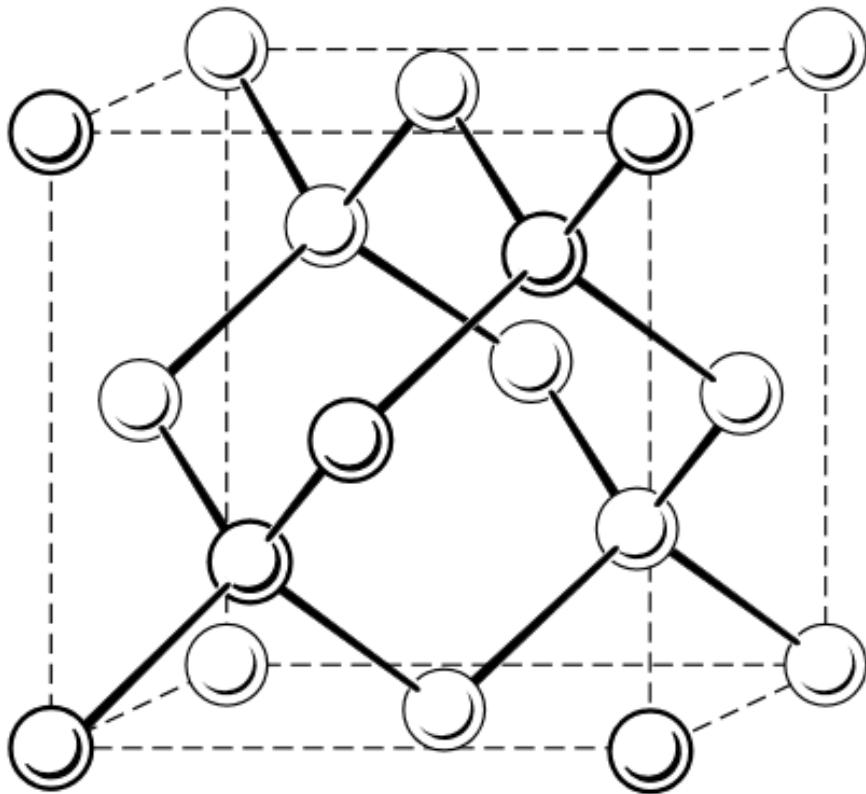


Figure 1.40 The diamond (zinc blende) crystal structure. From K. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

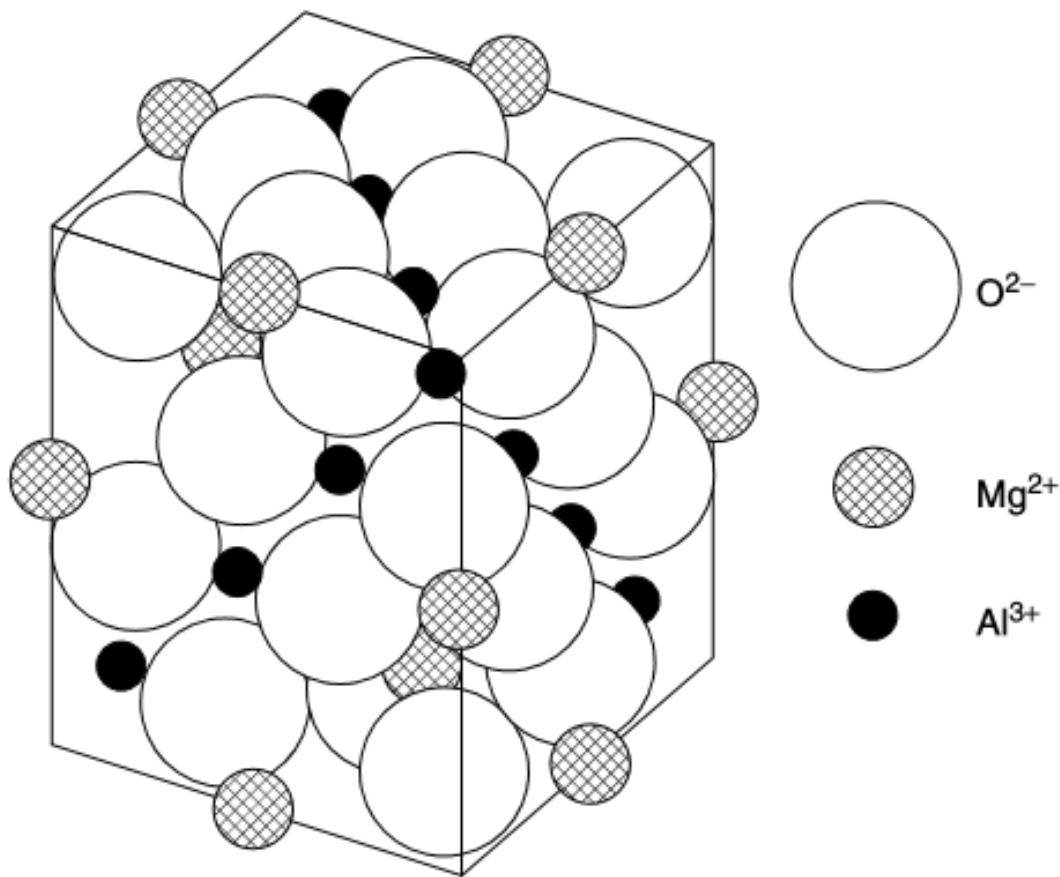
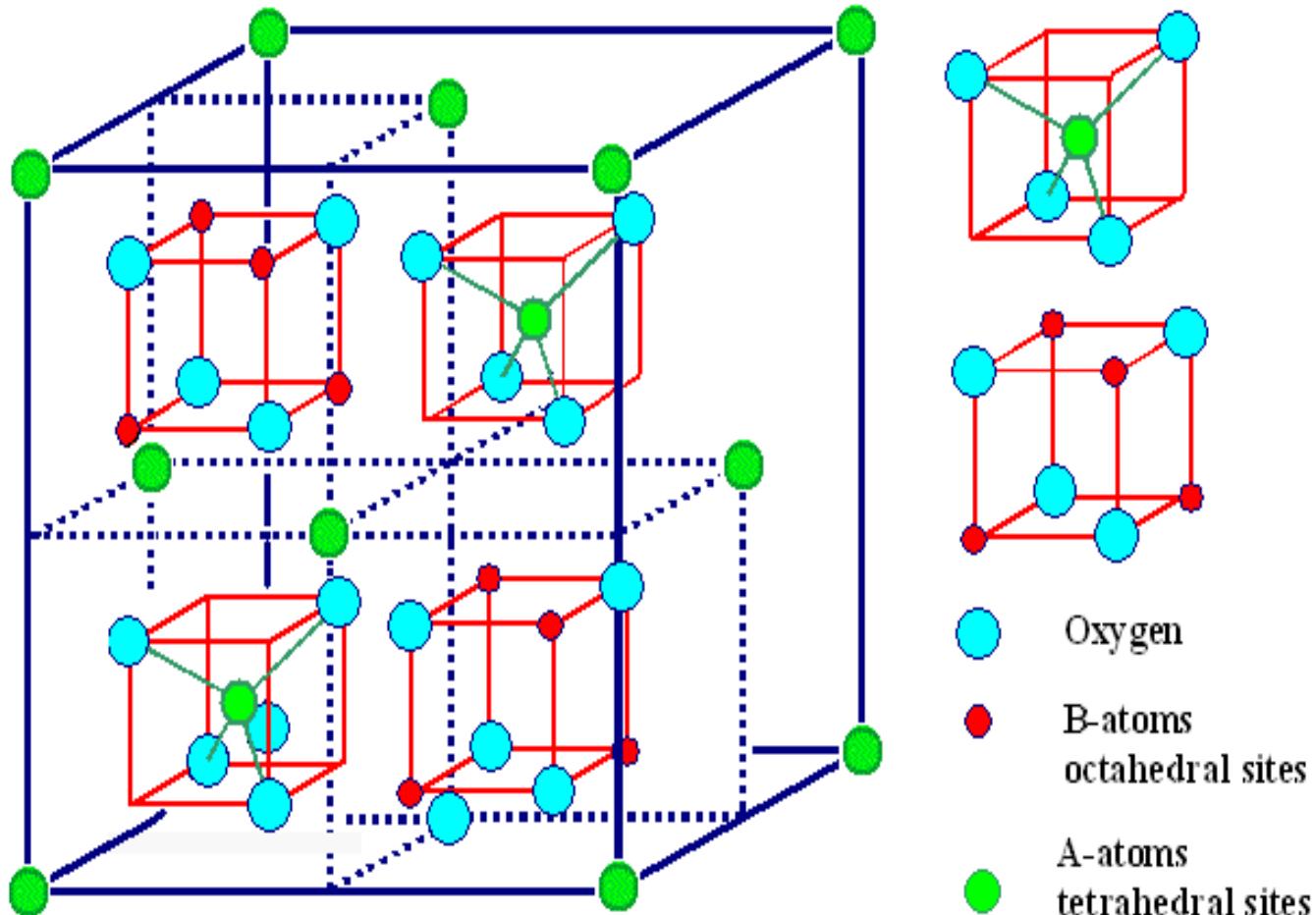


Figure 1.41 The spinel crystal structure of MgAl_2O_4 . Reprinted, by permission, from C. Kittel, *Introduction to Solid State Physics*, p. 447. Copyright © 1957 by John Wiley & Sons, Inc.



AB_2O_4 spinel The red cubes are also contained in the back half of the unit cell

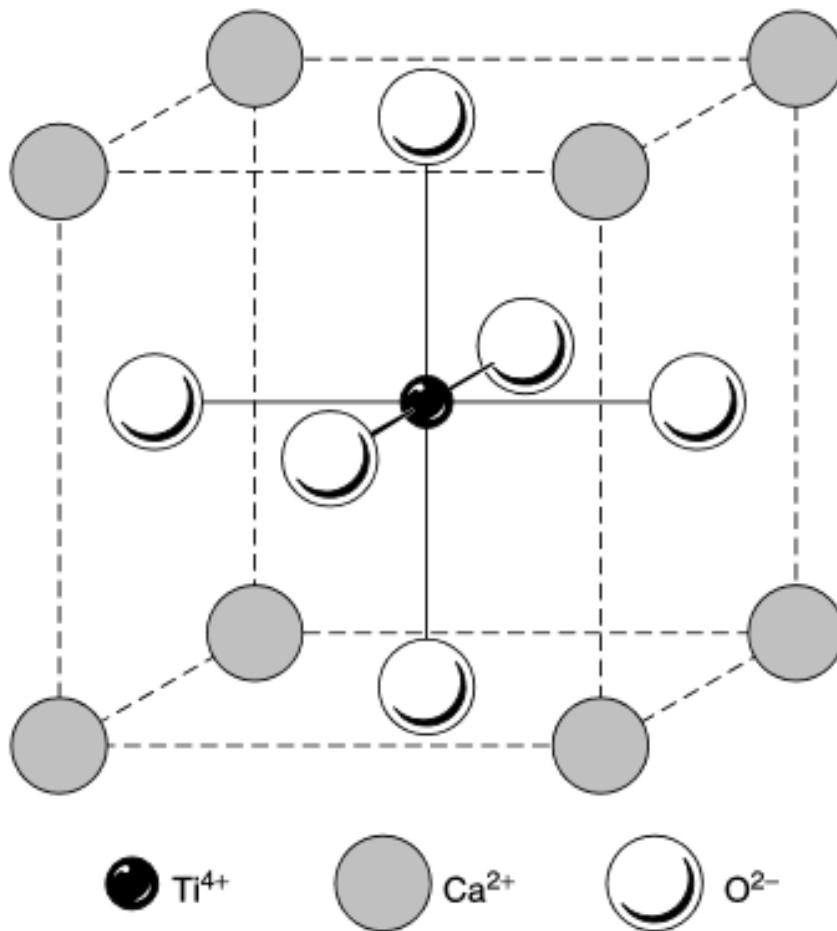
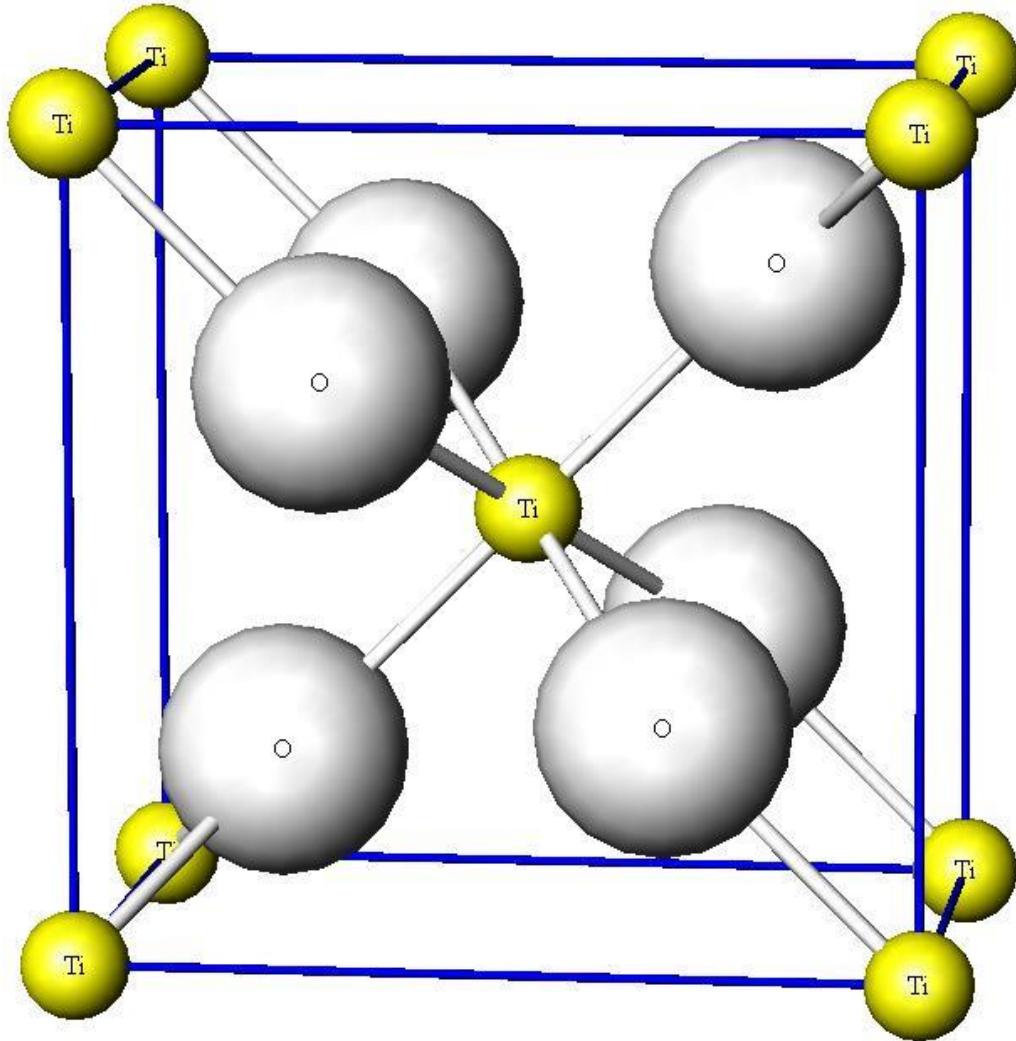
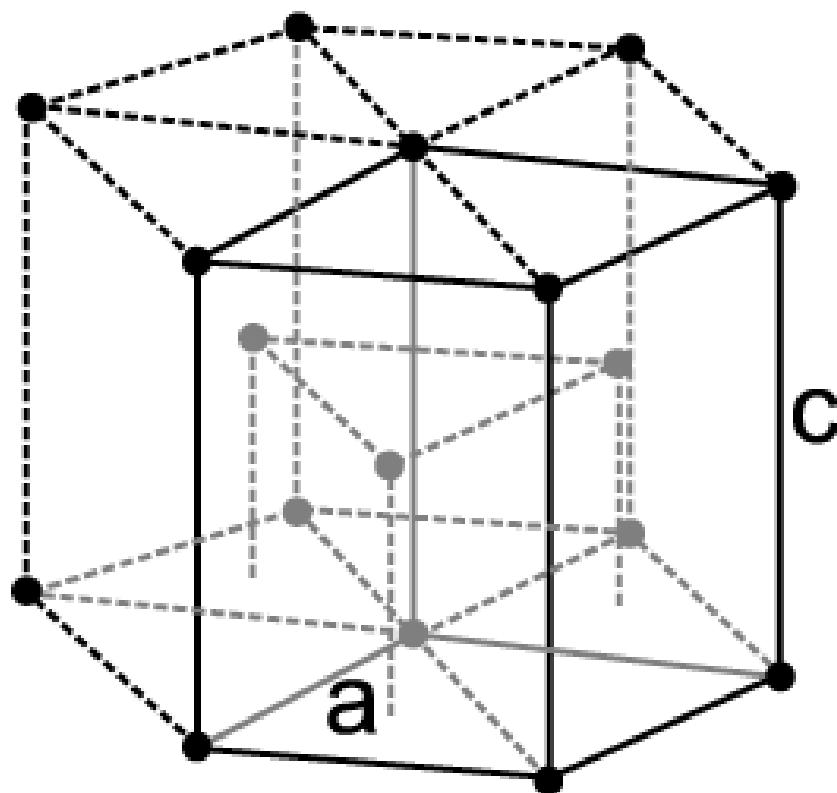


Figure 1.42 The perovskite crystal structure of CaTiO_3 . From W. D. Kingery, H. K. Bowen, and D. R. Uhlmann, *Introduction to Ceramics*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.



Rutile structure (TiO_2)



Hexagonal close packed (Corundum)

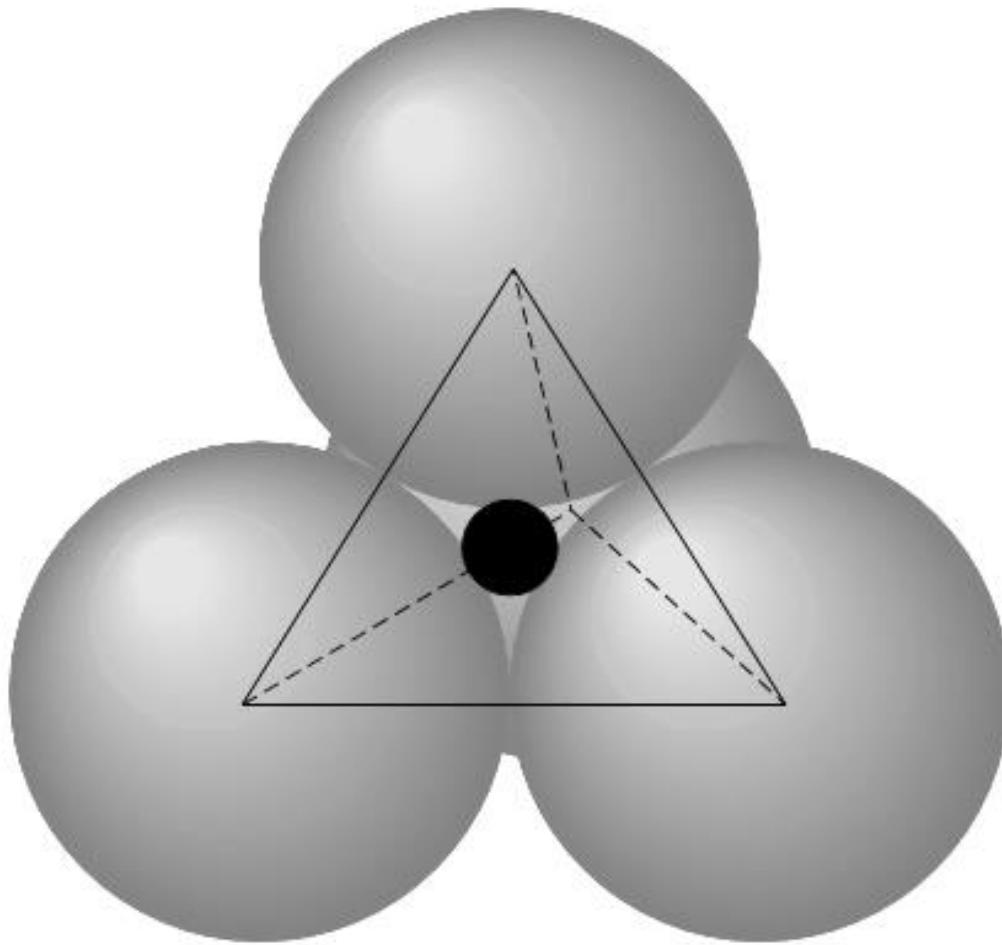


Figure 1.43 The $(\text{SiO}_4)^{4-}$ tetrahedron. The silicon atom is the solid circle at the center of the tetrahedron; large open circles are oxygens.

Table 1.17 Structural Units Observed in Crystalline Silicates

O/Si Ratio	Silicon–Oxygen		Examples
	Groups	Structural Units	
2	SiO_2	Three-dimensional network	Quartz
2.5	Si_4O_{10}	Sheets	Talc
2.75	Si_4O_{11}	Chains	Amphiboles
3.0	SiO_3	Chains, rings	Pyroxenes, beryl
3.5	Si_2O_7	Tetrahedra sharing one oxygen ion	Pyrosilicates
4.0	SiO_4	Isolated orthosilicate tetrahedra	Orthosilicates

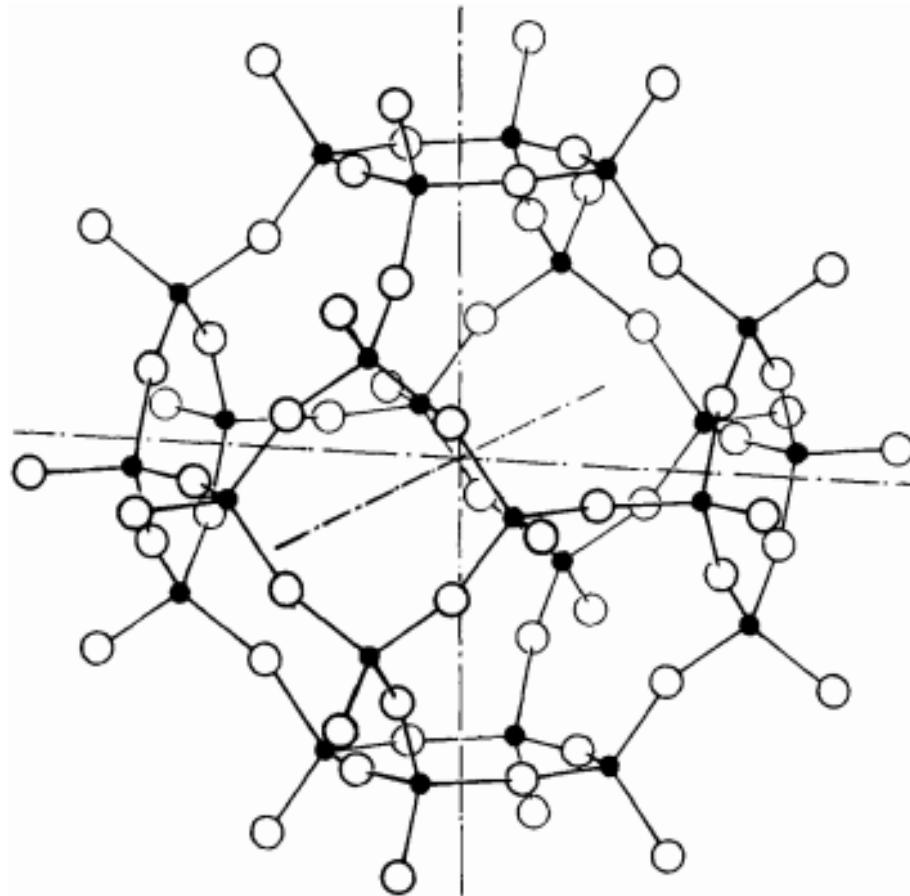


Figure 1.44 The structure of quartz, showing the three-dimensional network of SiO_4 tetrahedra. Reprinted, by permission, from L. G. Berry, B. Mason, and R. V. Dietrich, *Mineralogy: Concepts, Descriptions, Determinations*, p. 388, 2nd ed. Copyright © 1983, Freeman Publishing, Inc.

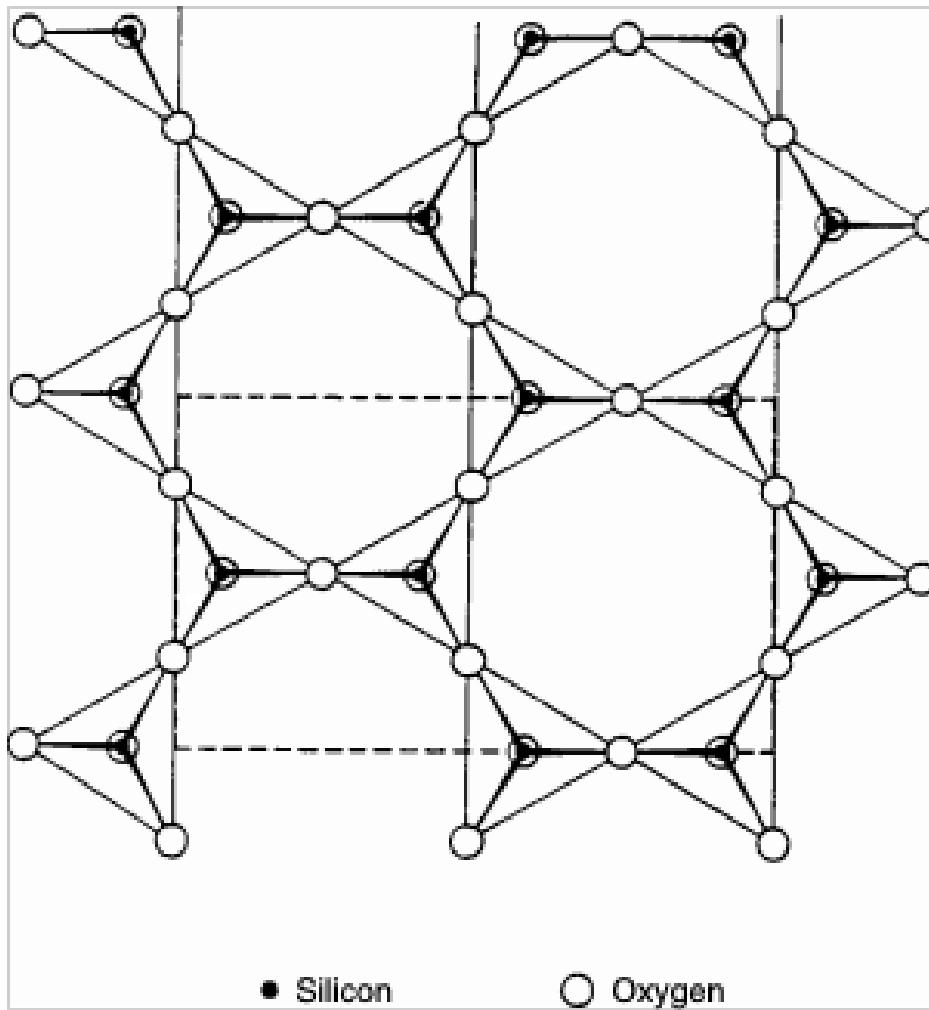


Figure 1.45 Top view of a silicate sheet structure resulting from sharing three corners of the SiO_4 tetrahedra. From W. D. Kingery, H. K. Bowen, and D. R. Uhlmann, *Introduction to Ceramics*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

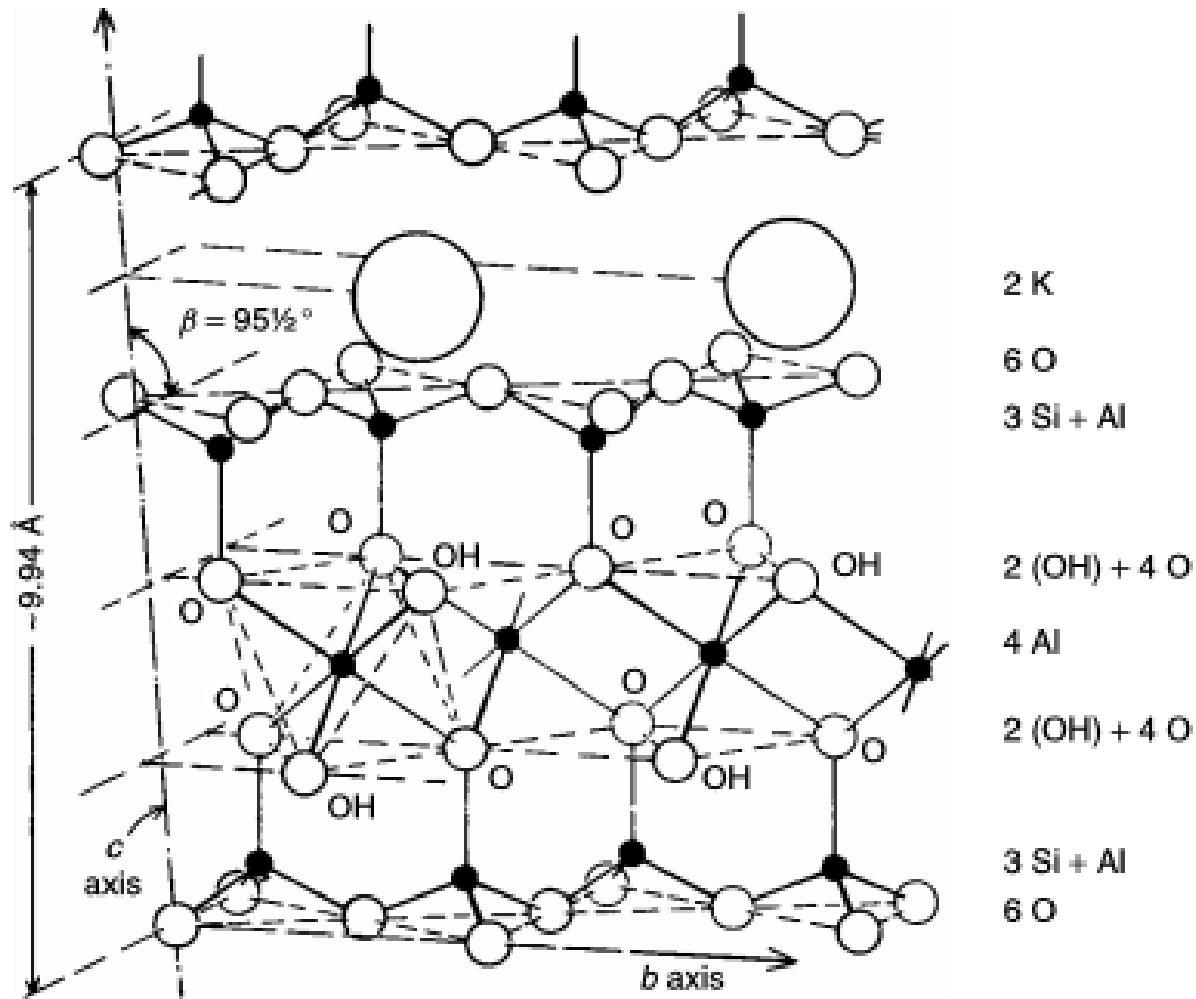


Figure 1.46 The structure of muscovite (mica), a sheet silicate. Reprinted, by permission, from L. G. Berry, B. Mason, and R. V. Dietrich, *Mineralogy: concepts, descriptions, determinations*, p. 431, 2nd ed. Copyright © 1983 by Freeman Publishing, Inc.

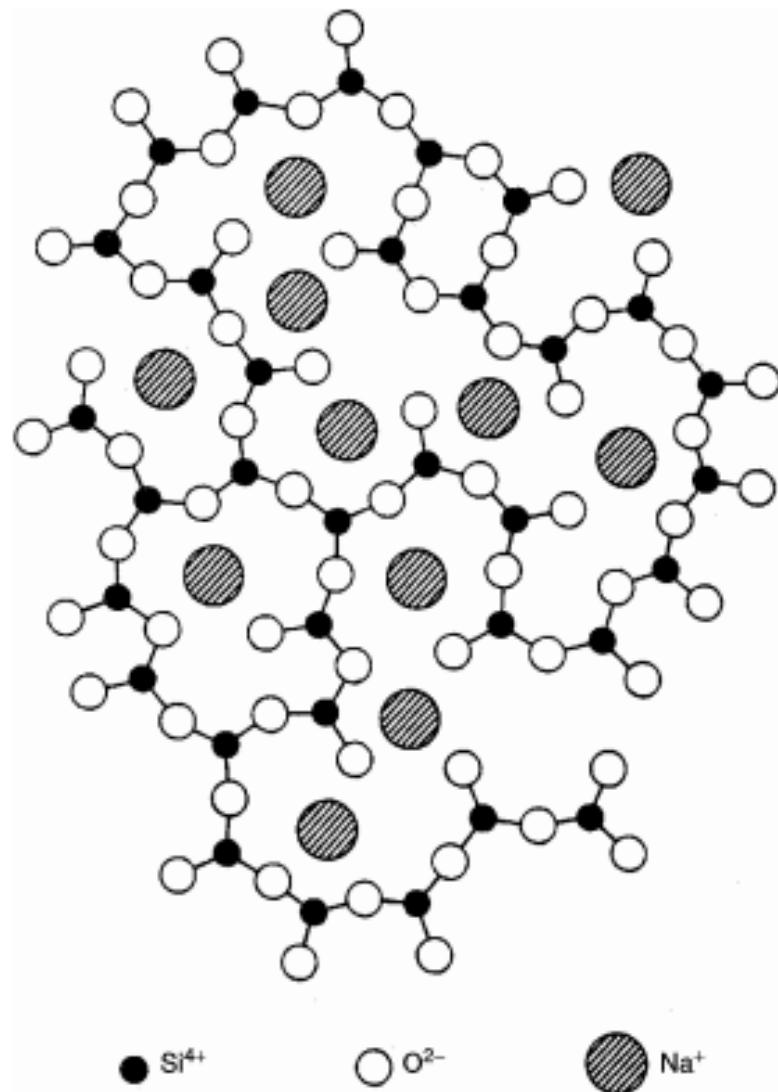


Figure 1.48 Schematic representation of a random network sodium silicate glass. From W. D. Kingery, H. K. Bowen, and D. R. Uhlmann, *Introduction to Ceramics*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

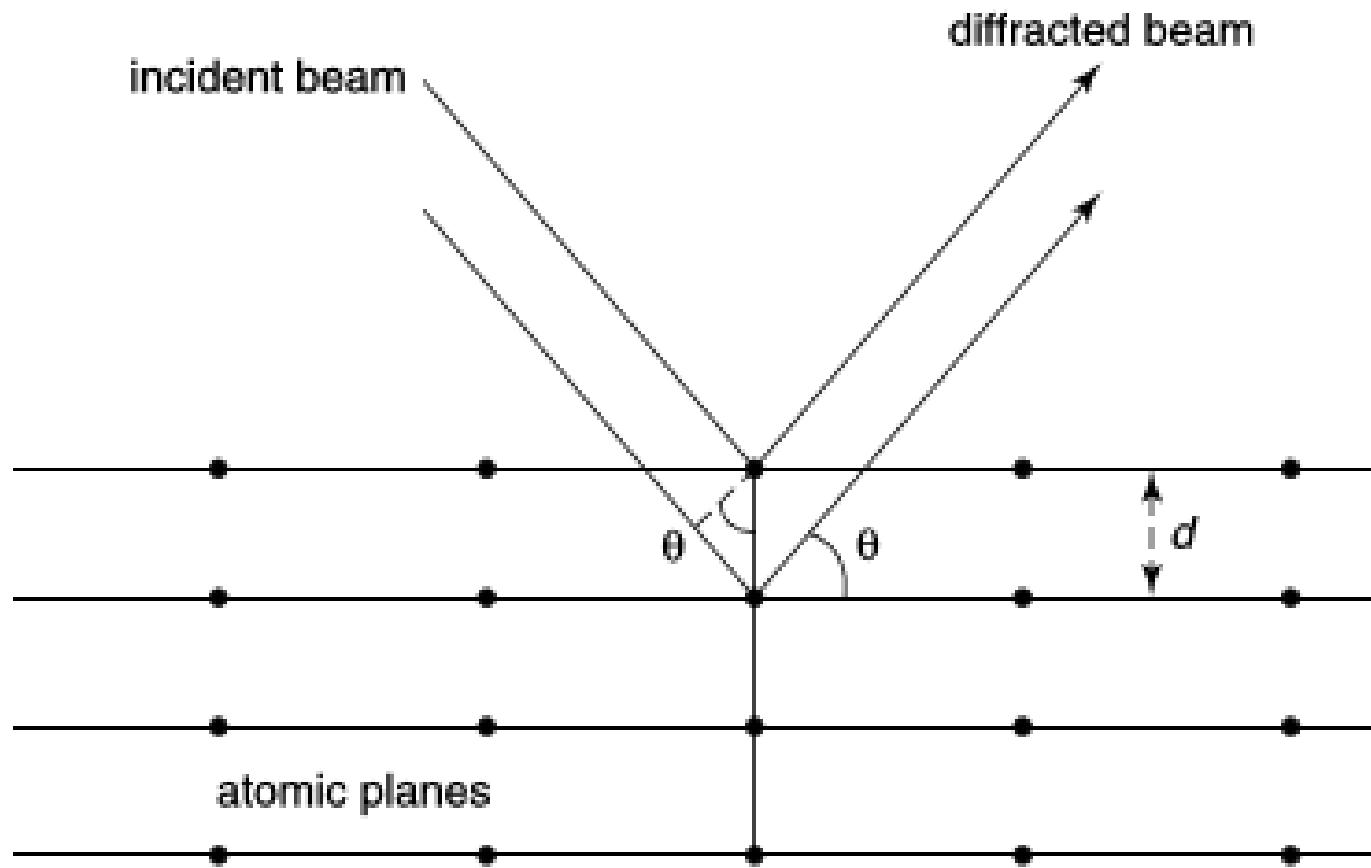


Figure 1.26 Schematic illustration of incident radiation diffraction by a crystal lattice.

$$n\lambda = 2d \sin \theta$$

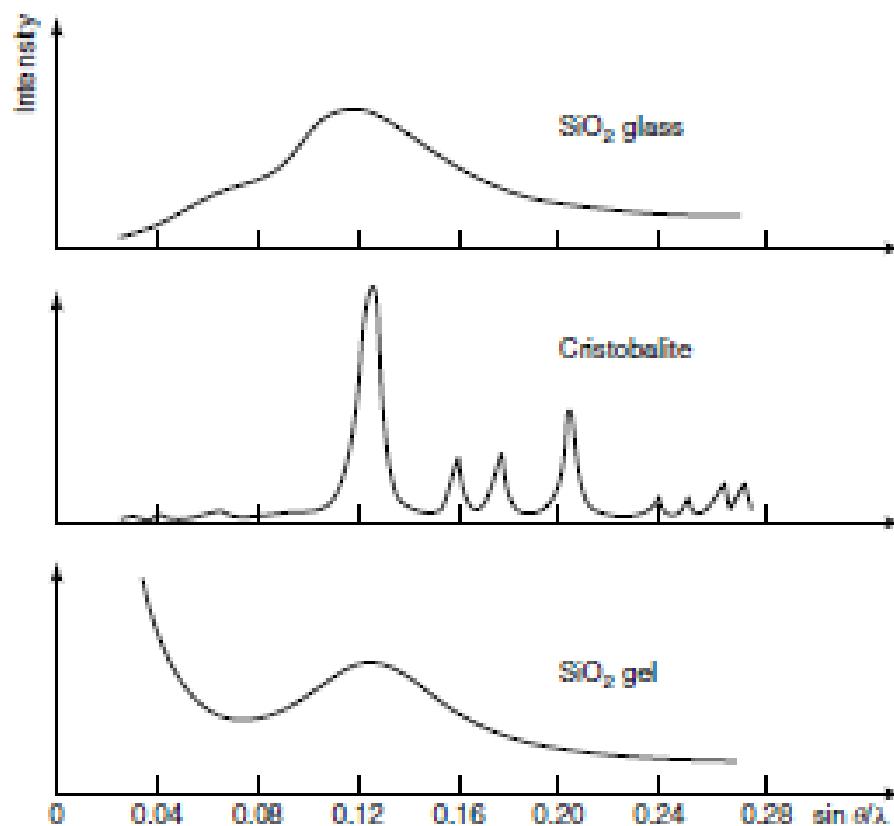


Figure 1.50 X-ray diffraction patterns of vitreous silicon, crystalline silica (cristobalite), and sol-gel-derived silica. Reprinted, by permission from H. Scholze, *Glass*, p. 97. Copyright © 1991 by Springer-Verlag.

$$\text{rdf} = 4\pi r^2 n_0 g(r)$$

where $g(r)$ is the pair distribution function between adjacent atoms—that is, the probability of finding another atom a distance r from the reference atom located at $r = 0$ and n_0 is the average number density = N/V

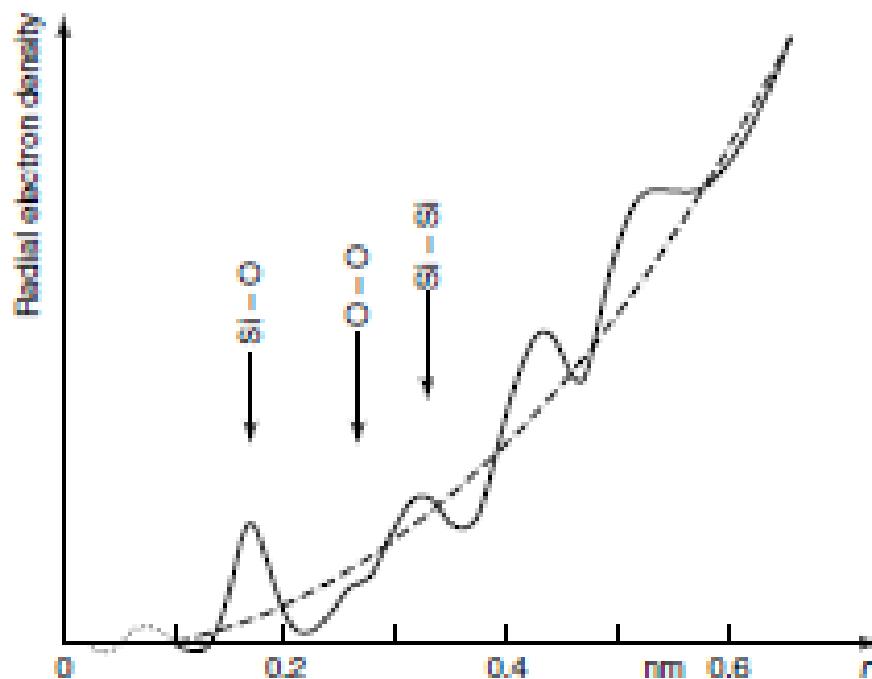


Figure 1.51 Radial distribution of electron densities of vitreous silica from X-ray exposures (Scholze). Reprinted, by permission, from Scholze, H., *Glass*, p. 98. Copyright © 1991 by Springer-Verlag.

Zachariasen Rules 1932

Four rules for the formation of oxide glasses

- An anion (oxygen atom) is linked to not more than two glass-forming cations (metal atoms).
- The coordination numbers of the glass-forming atoms (cations) is small, four or less.
- The oxygen polyhedra (structural units) share corners with each other, not edges or faces.
- The polyhedra are linked in a 3-D network (at least three corners of each polyhedra should be shared).

Zachariasen's rules, as supported and modified by Warren, came to be known as the **random network theory**

Table I.20 The Alkane Series

Substance	Molecular Weight	T _m (°C)	T _f (°C)
Methane, CH ₄	16.04	-182.5	-164
Ethane, C ₂ H ₆	30.07	-183.3	-88.6
Propane, C ₃ H ₈	44.10	-189.7	-42.1
Butane, C ₄ H ₁₀	58.13	-138.4	-0.5
Pentane, C ₅ H ₁₂	72.15	-129.7	36.1
Hexane, C ₆ H ₁₄	86.18	-94.3	69.0
Heptane, C ₇ H ₁₆	100.21	-90.6	98.4
Octane, C ₈ H ₁₈	114.23	-56.8	125.7
Nonane, C ₉ H ₂₀	128.26	-53.7	150.8
Decane, C ₁₀ H ₂₂	142.29	-29.7	174.1

Table 1.21 Summary of Chain and Cyclic Hydrocarbons

Hydrocarbons	Formula	Characteristics
Chain		
Alkane series	C_nH_{2n+2}	All single C—C bonds
Alkene series	C_nH_{2n}	One double C=C bond
Alkadiene series	C_nH_{2n-2}	Two double C=C bonds
Alkyne series	C_nH_{2n-2}	One triple C≡C bond
Alkadiyne series	C_nH_{2n-6}	Two triple C≡C bonds
Cyclic		
Cycloalkane series	C_nH_{2n}	All single C—C bonds, cyclic
Cycloalkene series	C_nH_{2n-2}	One double C=C bond, cyclic
Aromatic	Various	Ring structures, based on the benzene ring, in which single and double carbon bonds alternate

Table 1.22 Some of the More Important Functional Groups in Polymer Chemistry

Group	General Formula	Compound Class	Example
—Cl	R—Cl	Chlorides	Methyl chloride, CH_3Cl
—OH	R—OH	Alcohols	Ethyl alcohol, $\text{CH}_3\text{CH}_2\text{OH}$
	$\text{R—C}(\text{=O})\text{—OH}$	Acids (or carboxylic acids)	Acetic acid, CH_3COOH
	$\text{R}_2\text{C=O}$	Ketones	Acetone, CH_3COCH_3
	$\text{H}\text{C=O}\text{R}$	Aldehydes	Propionaldehyde, $\text{CH}_3\text{CH}_2\text{CHO}$
—O—	R—O—R	Ethers	Ethyl ether, $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$
—NH_2	R—NH_2	Amines	Propylamine, $\text{CH}_3(\text{CH}_2)_2\text{NH}_2$
	$\text{R—C}(\text{=O})\text{—NH}_2$	Amides	Acetamide, CH_3CONH_2
	$\text{R—C}(\text{=O})\text{—O—R'}$	Esters	Ethyl acetate, $\text{CH}_3\text{COOC}_2\text{H}_5$

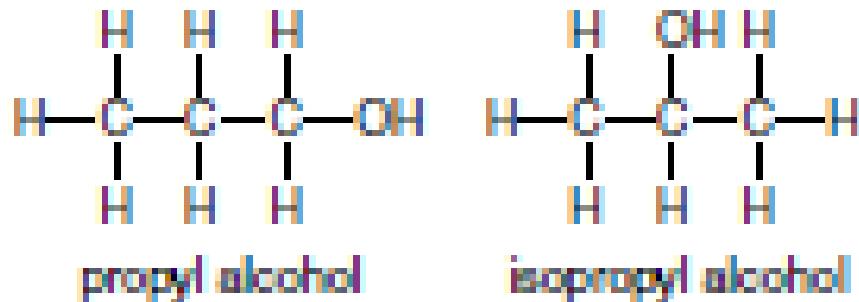


Figure 1.53 An example of polymer structural isomers.

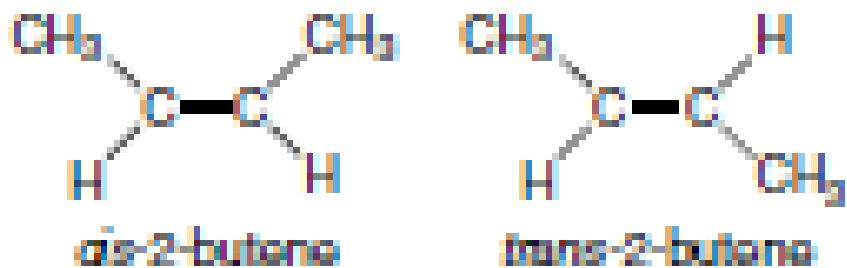


Figure 1.54 An example of polymer stereoisomers.

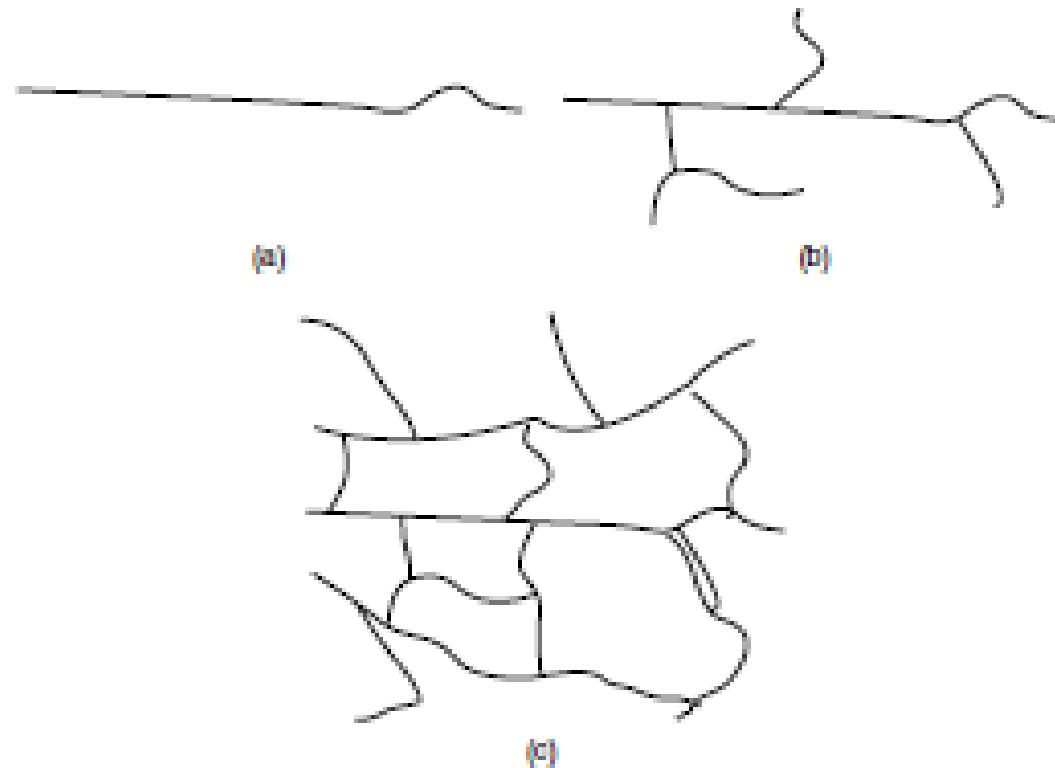


Figure 1.55 Classification of polymers according to macroscopic structure: (a) linear, (b) branched and (c) networked.

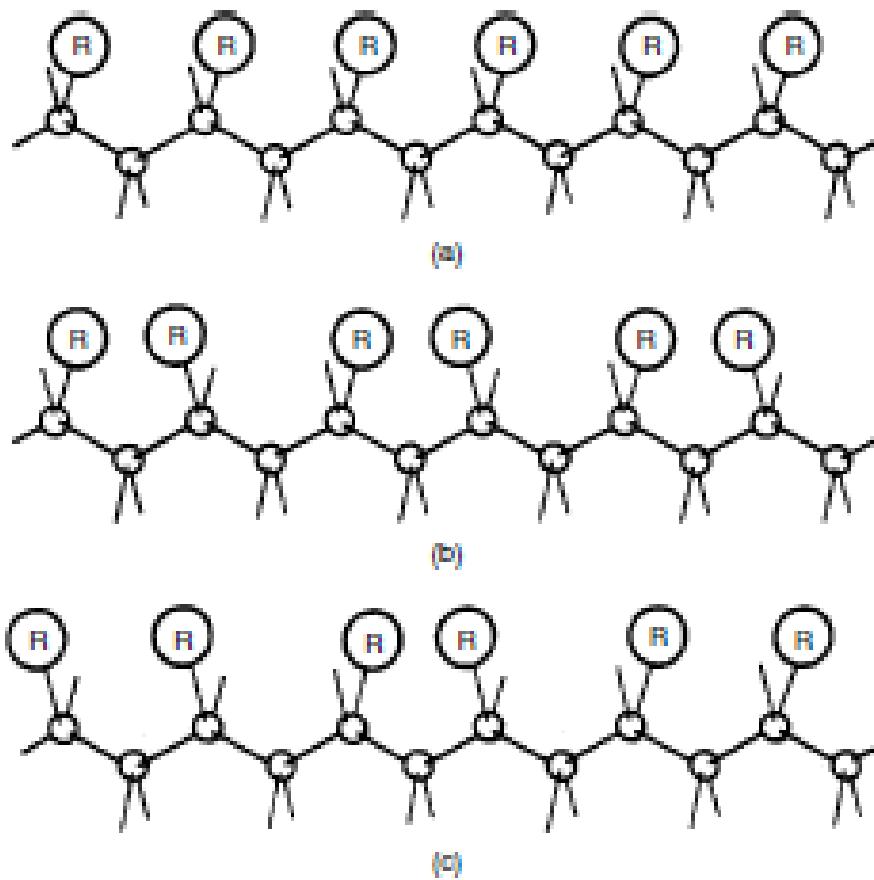


Figure 1.57 Summary of different types of tacticity, where R represents an atom other than hydrogen: (a) isotactic; (b) syndiotactic; and (c) atactic. Reprinted, by permission, from P. Hiemenz, *Polymer Chemistry: The Basic Concepts*, p. 27. Copyright © 1984 by Marcel Dekker, Inc.

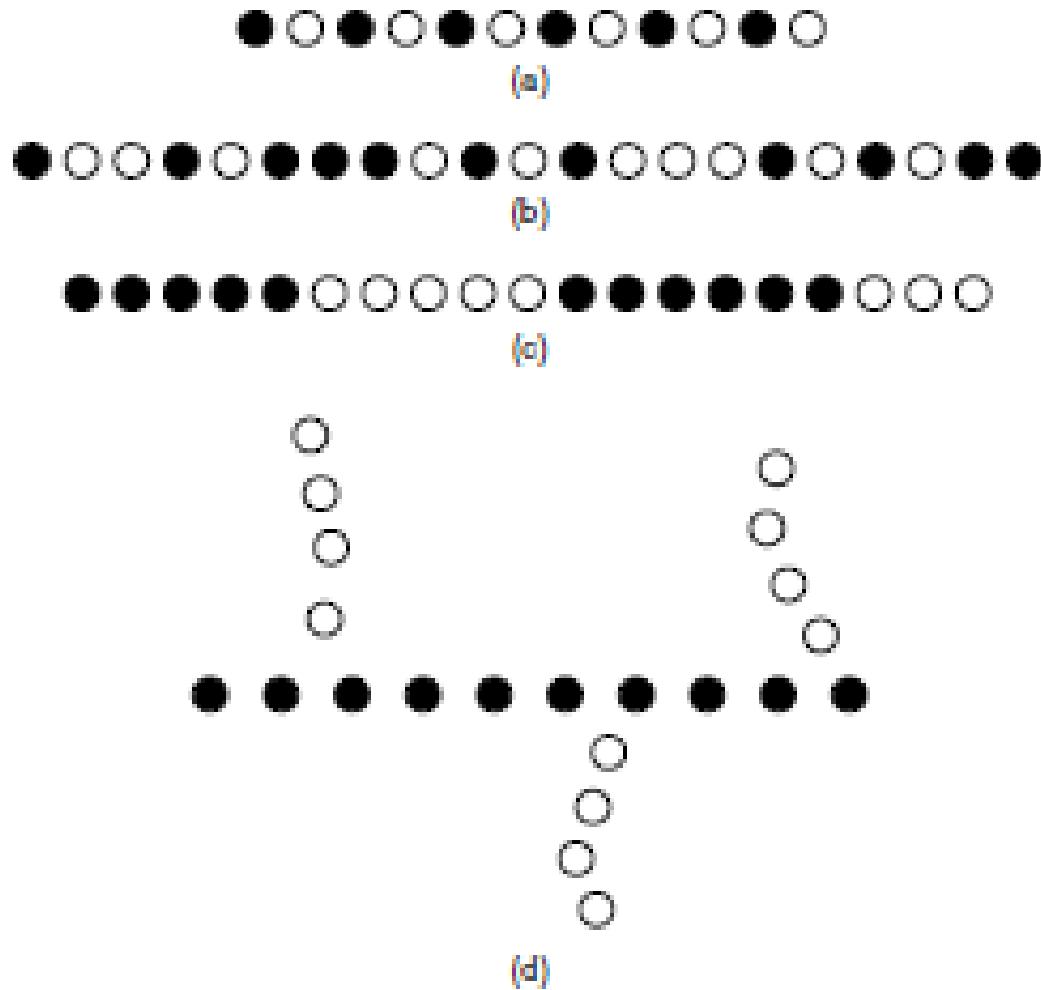


Figure 1.58 Summary of copolymer classifications: (a) alternating, (b) random, (c) block, and (d) graft.



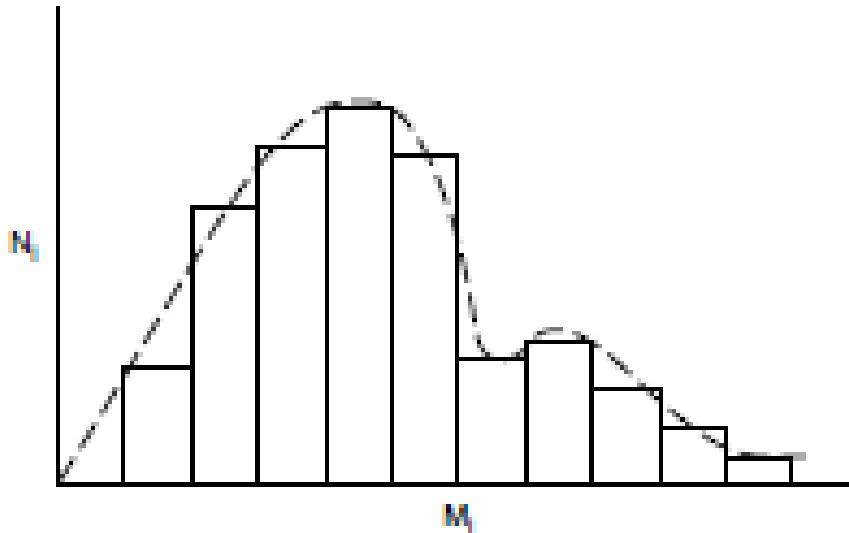


Figure 1.59 Histogram showing the number of molecules, N_i , having the molecular weight M_i . Reprinted, by permission, from P. Heimenz, *Polymer Chemistry: The Basic Concepts*, p. 35. Copyright © 1984 by Marcel Dekker, Inc.

Table 1.23 Summary of the Most Common Molecular Weight Averages

Average	Definition	Methods of Determination
\overline{M}_n	$\frac{\sum N_i M_i}{\sum N_i}$	Osmotic pressure, colligative properties, end group analysis
\overline{M}_w	$\frac{\sum N_i M_i^2}{\sum N_i M_i}$	Light scattering, sedimentation velocity
\overline{M}_z	$\frac{\sum N_i M_i^3}{\sum N_i M_i^2}$	Sedimentation equilibrium
\overline{M}_v	$\left(\frac{\sum N_i M_i^{1+\alpha}}{\sum N_i M_i} \right)^{1/\alpha}$	Intrinsic viscosity (α is characteristic of a system and lies between 0.5 and 1.0)

$$\frac{\overline{M}_w}{\overline{M}_n} \geq 1.0$$

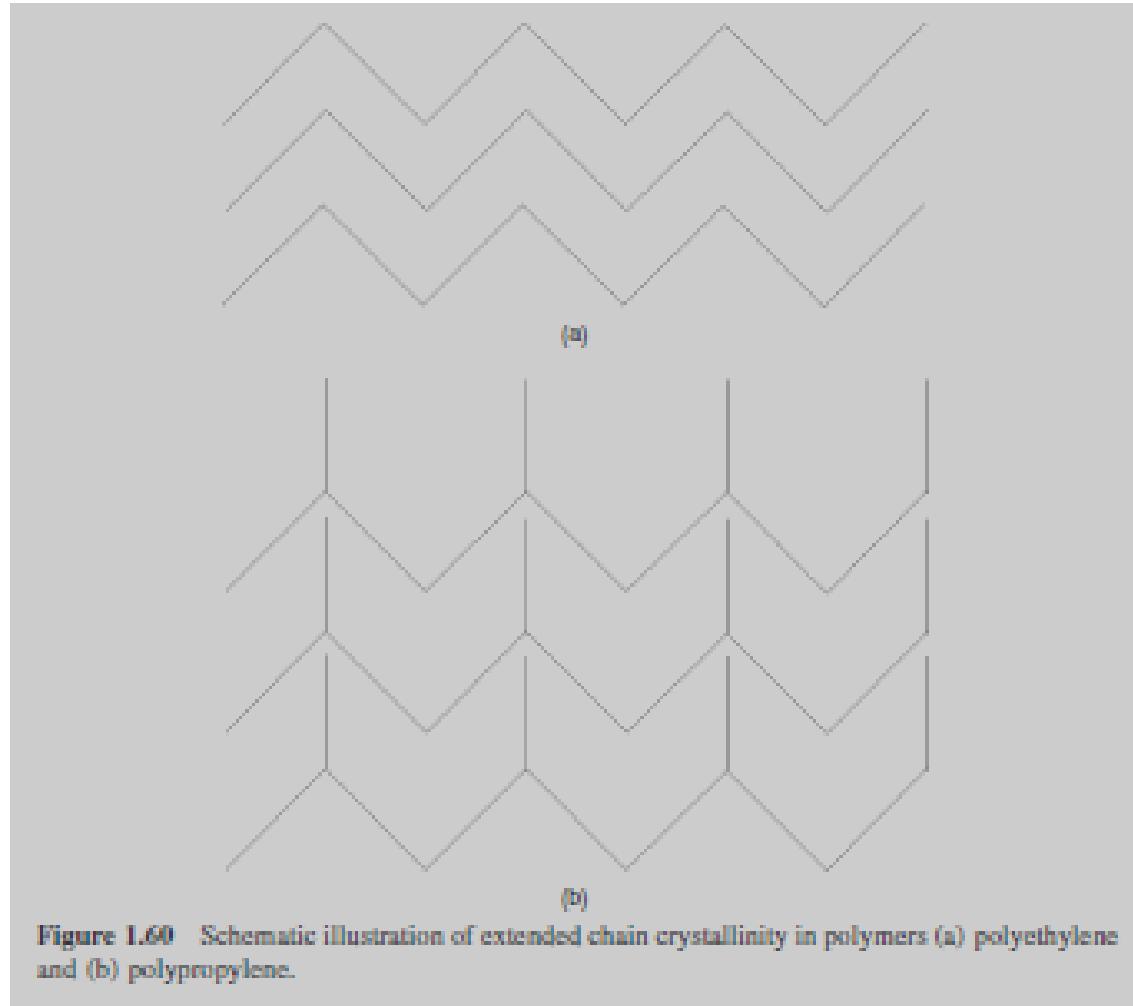


Figure 1.60 Schematic illustration of extended chain crystallinity in polymers (a) polyethylene and (b) polypropylene.

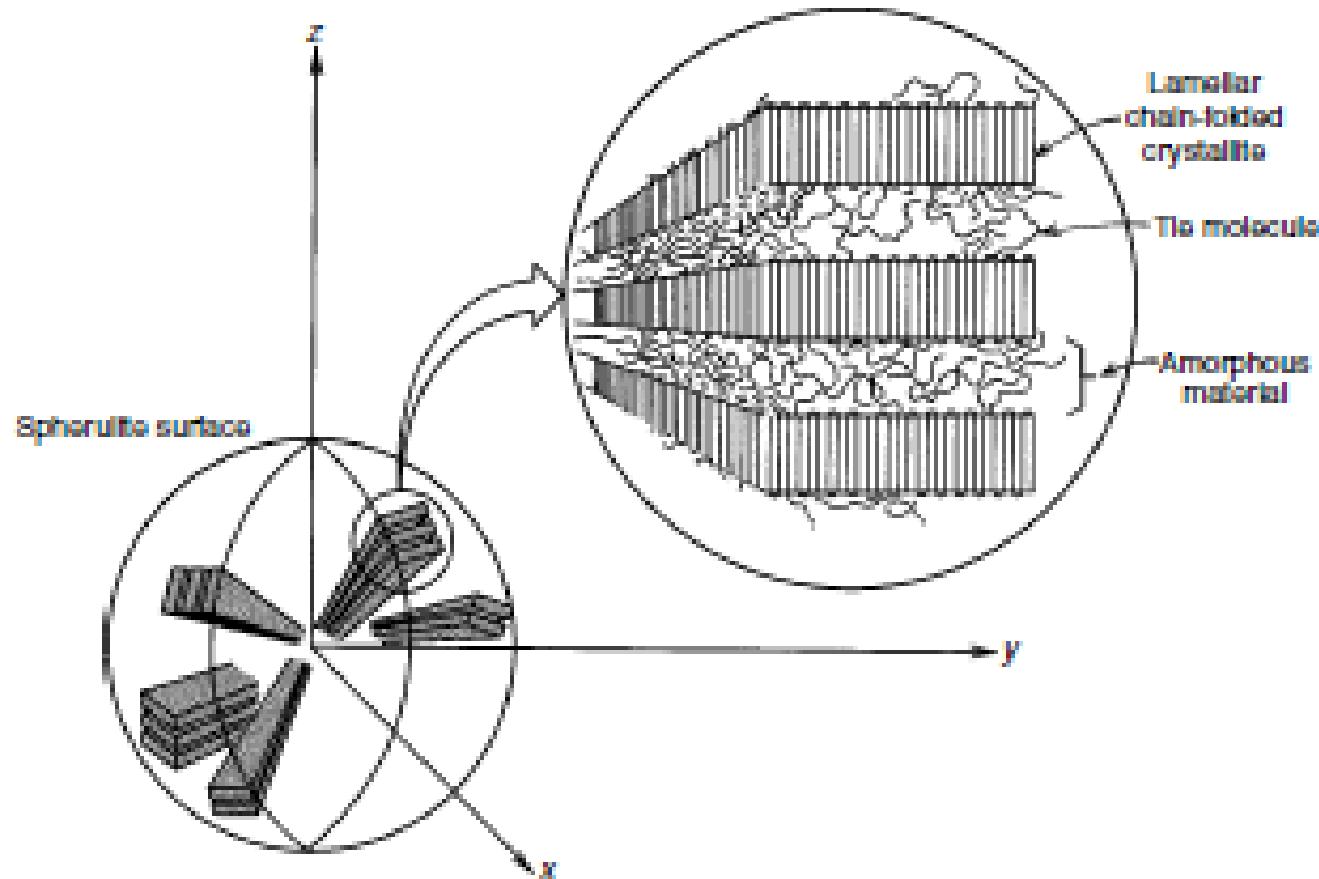


Figure 1.61 Schematic illustration of chain folding leading to lamellar crystallites (inset) and lamellar stacking to form spherulites.

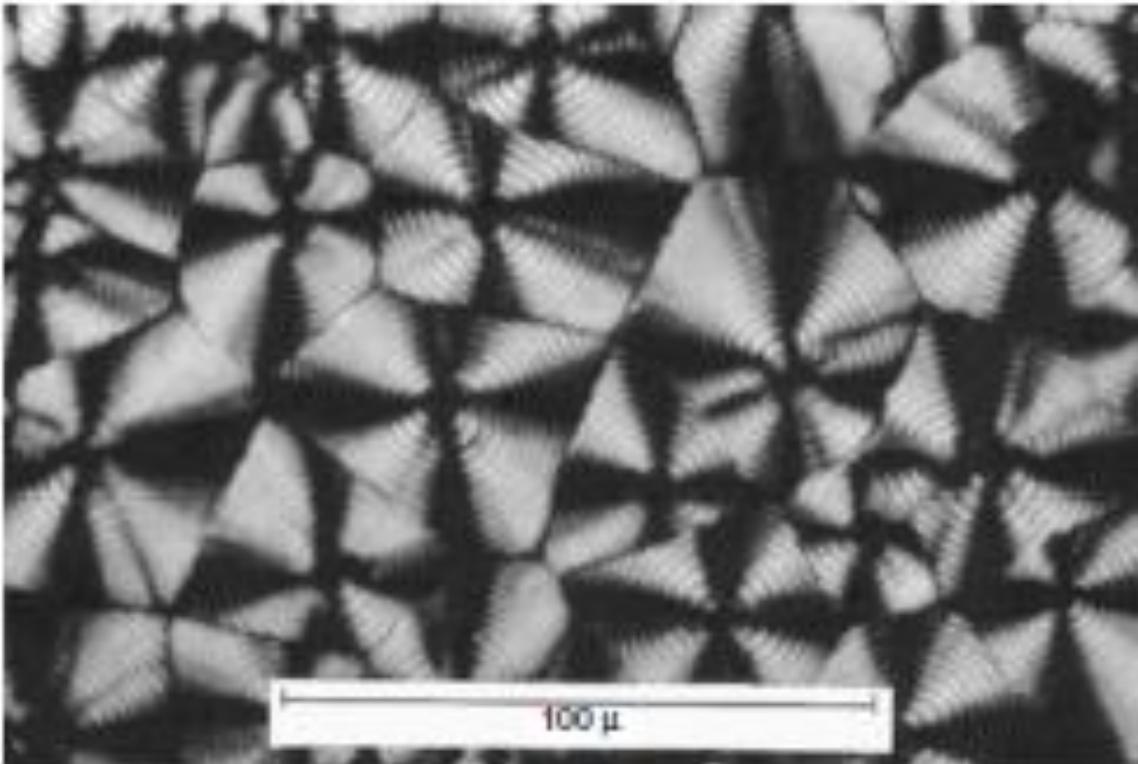


Figure 1.62 Cross-polarized micrograph of polyethylene showing spherulitic structure. From K. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

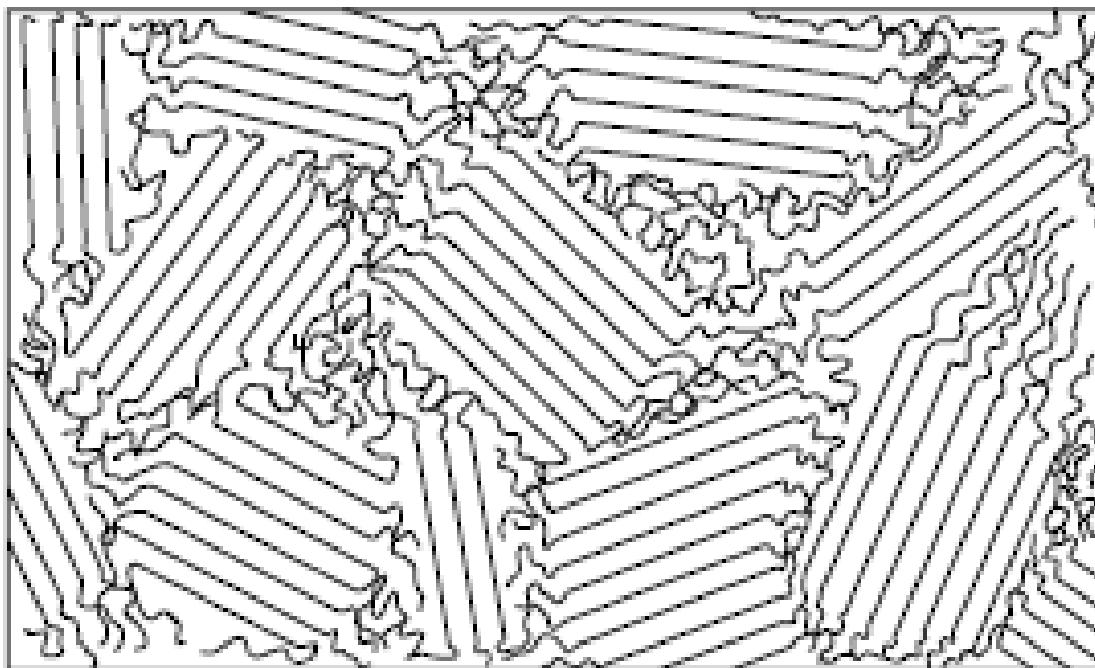


Figure 1.63 The fringed-micelle model of polymer crystallinity. From K. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.



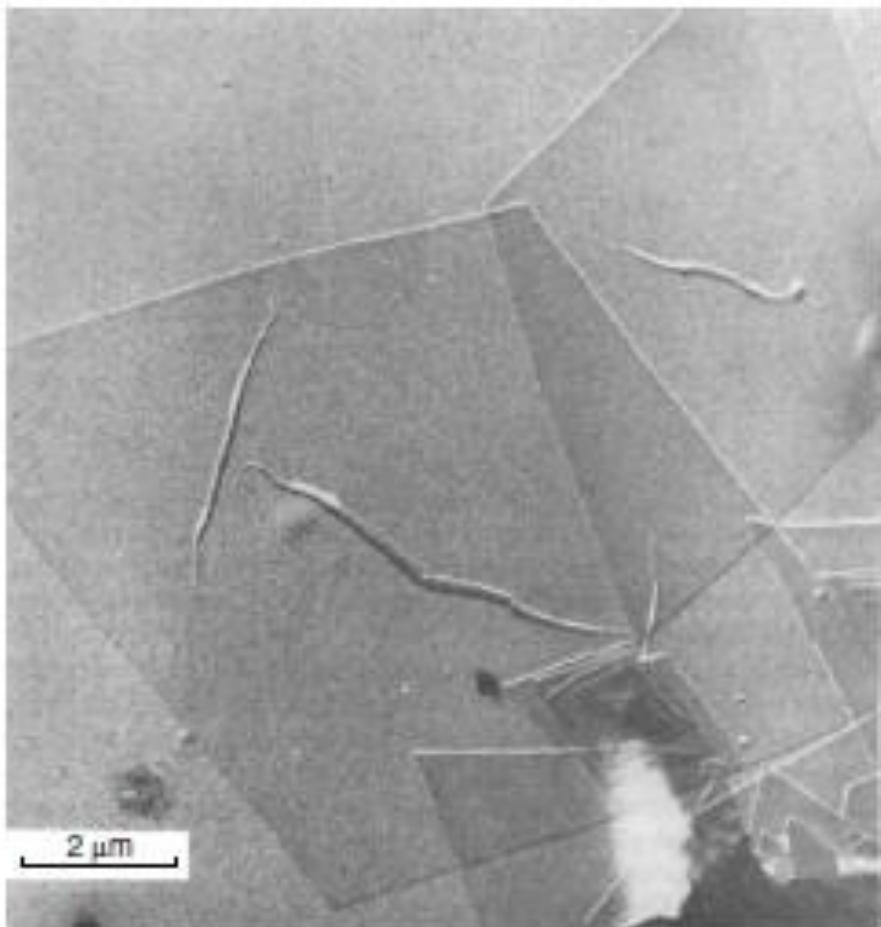


Figure 1.64 Polyethylene single crystals. Reprinted, by permission, from P. Heimenz, *Polymer Chemistry: The Basic Concepts*, p. 239. Copyright © 1984 by Marcel Dekker, Inc.

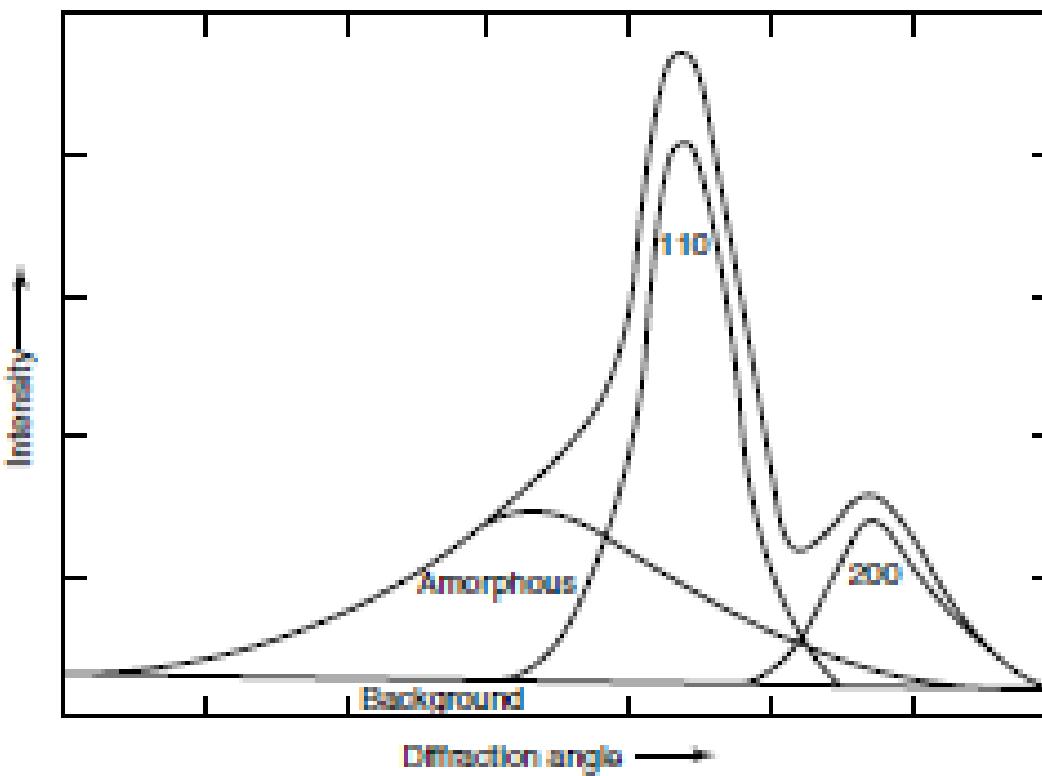


Figure 1.66 Resolution of the X-ray scattering curve of a semicrystalline polyethylene sample into contributions from crystalline (110 and 200 planes) and amorphous components. From F. W. Billmeyer, *Textbook of Polymer Science*, 3rd ed. Copyright © 1984 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

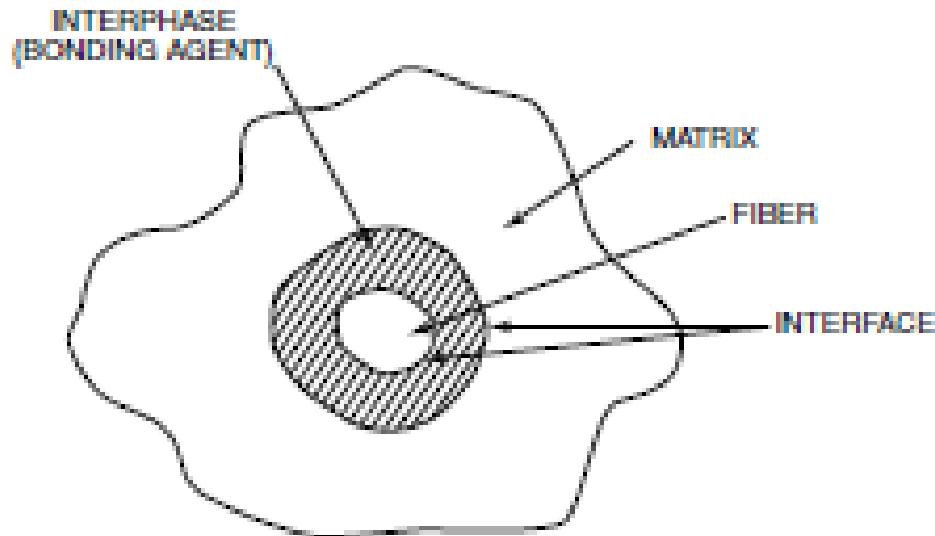
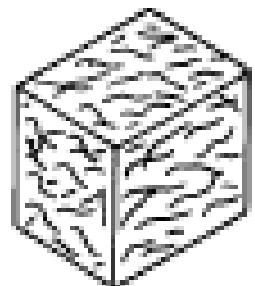
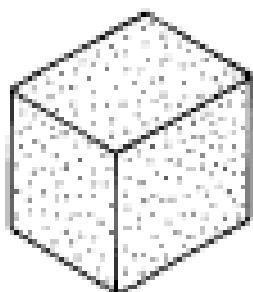


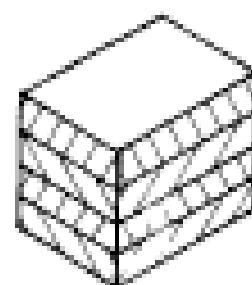
Figure 1.73 Schematic illustration of composite constituents. Reprinted, by permission, from M. Schwartz, *Composite Materials Handbook*, 2nd ed., p. 1.4. Copyright © 1992 by McGraw-Hill.



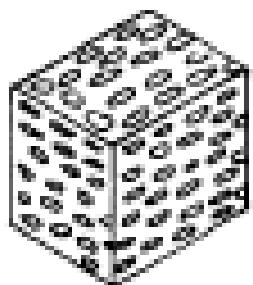
FIBER COMPOSITE



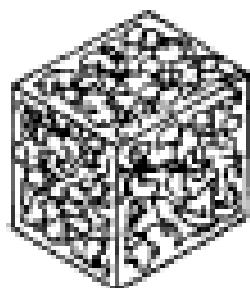
PARTICULATE COMPOSITE



LAMINAR COMPOSITE



FLAKE COMPOSITE



FILLED COMPOSITE

Figure 1.74 Classes of composites. Reprinted, by permission, from Schwartz, M., *Composite Materials Handbook*, 2nd ed., p. 1.7. Copyright © 1992 by McGraw-Hill.

Table 1.28 Some Typical Polymers Used as Matrices in PMCs

Matrix Material	Process Temperature (°C)	Upper Use Temperature (°C)
<i>Thermosetting</i>		
Polyester (phthalic/maleic type)	RT	70
Vinyl ester	RT	125
Epoxy	150	125
Epoxy	200	175
Phenolic	250	200
Cyanates (triazines)	250	200
Bismaleimides	250	225
Nadic end-capped polyimides (e.g., PMR-15)	316	316
<i>Thermoplastic</i>		
Polysulfone	325	180
Polyamide	250	100
Polycarbonate	280	100
Polyphenylene oxide (PPO)	280	100
Polysulfides (PPS)	300	150
Polyether ether ketone (PEEK)	370	175
Polyether sulfone (PES)	350	175
Polyamide-imides	325	200
Polyetherimide	400	275
Polyimide	370	316
Polyarylate	400	300
Polyester (liquid crystalline)	300	150

Table 1.29 Common Metals for Metal-Matrix Composites

Matrix Material	Fabrication Method	Typical Composite Density (g/cm ³)	Use Temperature (°C)
Aluminum	Diffusion bonding		350
	Hot molding	2.62–3.45	
	Powder metallurgy		
	Liquid processing		
Magnesium	Liquid processing	1.82–2.80	300
	Diffusion bonding		
Titanium	Diffusion bonding	3.76–4.00	650
Iron-, nickel-based alloys	Diffusion bonding	5.41–11.7	800–1150

Table 1.30 Common Ceramics for Ceramic-Matrix Composites

Matrix Material	Density (g/cm ³)	Use Temperature (°C)
Alumina, Al ₂ O ₃	4.0	~1000
Glass ceramics	2.7	900
Si ₃ N ₄	3.1	~1300
SiC	3.2	~1300

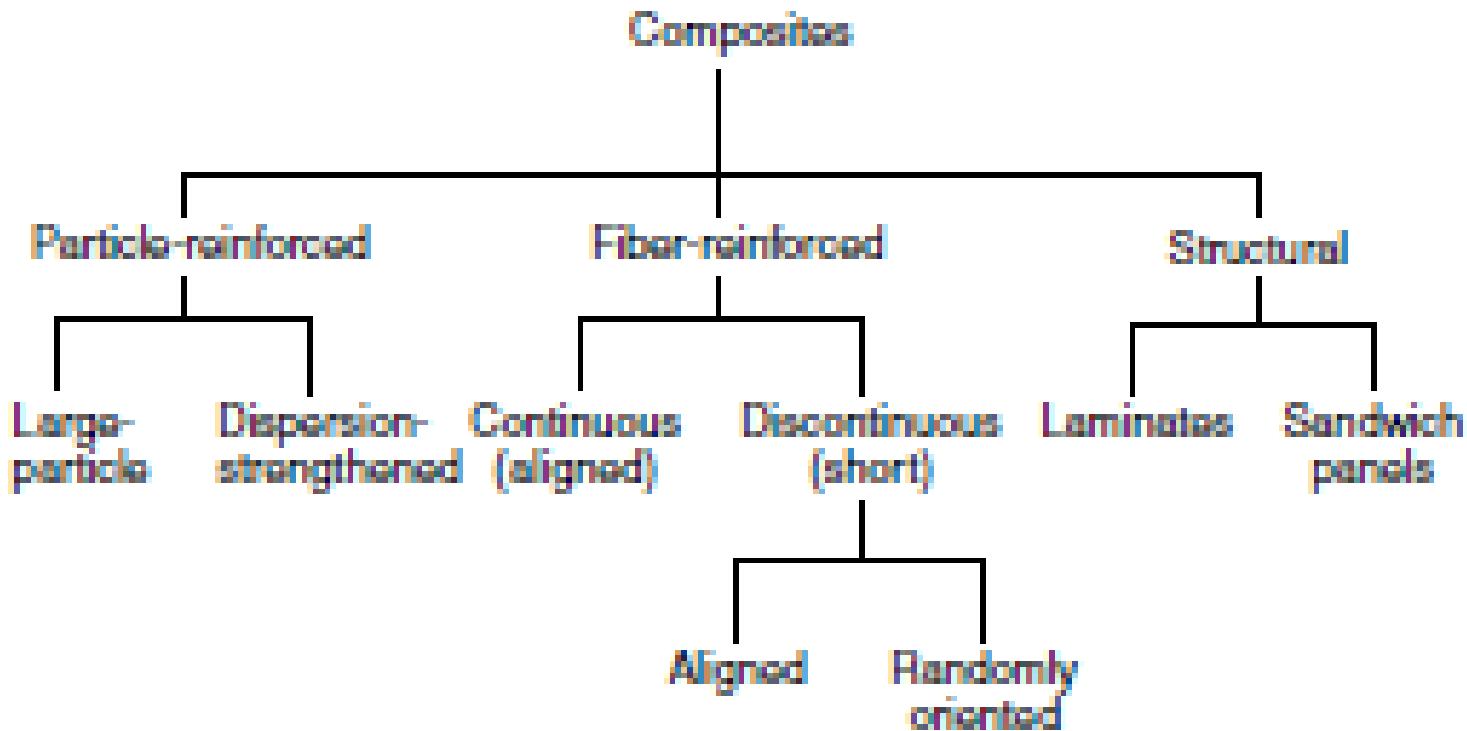
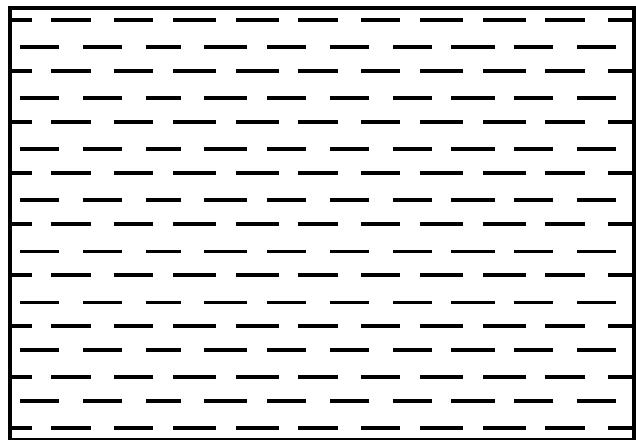
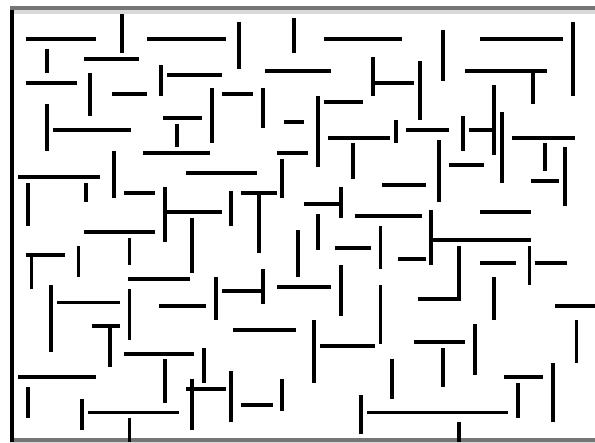


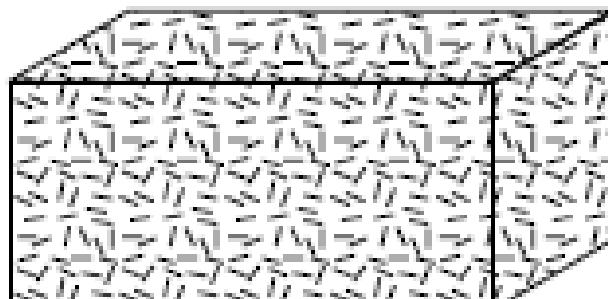
Figure 1.75 Types of reinforced composites.



(a)



(b)



(c)

Figure 1.76 Types of fiber reinforcement orientation (a) one-dimensional, (b) two-dimensional, and (c) three-dimensional.

Table 1.31 Selected Properties of Some Common Reinforcing Fibers

Fiber	Density (g/cm ³)	Melting Point (°C)	Specific Modulus (GPa · cm ³ /g)	Specific Strength (MPa · cm ³ /g)
Aluminum	2.70	660	27	230
Steel	7.87	1621	25	530
Tantalum	16.6	2996	12	37
Titanium	4.72	1668	24	410
Tungsten	19.3	3410	21	220
Boron	2.30	2100	192	1500
Beryllium	1.84	1284	165	710
Molybdenum	10.2	2610	35	140
Aluminum oxide	3.97	2082	132	170
Aluminosilicate	3.90	1816	26	1060
Asbestos	2.50	1521	60	550
Beryllium carbide	2.44	2093	127	420
Beryllium oxide	3.03	2566	116	170
Carbon	1.76	3700	114	1570
Graphite	1.50	3650	230	1840
E-glass	2.54	1316	28	1360
S-glass	2.49	1650	34	1940
Quartz	2.20	1927	32	407
SiC (on tungsten)	3.21	2316	140	1000
Si ₃ N ₄	2.50	1900	100	1344
BN	1.91	3000 (decomp.)	47	722
ZrO ₂	4.84	2760	71	427
Wood	0.4–0.8	—	17	—
Polyamide (Kevlar)	1.14	249	2.5	730
Polyester	1.40	249	2.9	490
Polypropylene	0.9	154	1.8	77

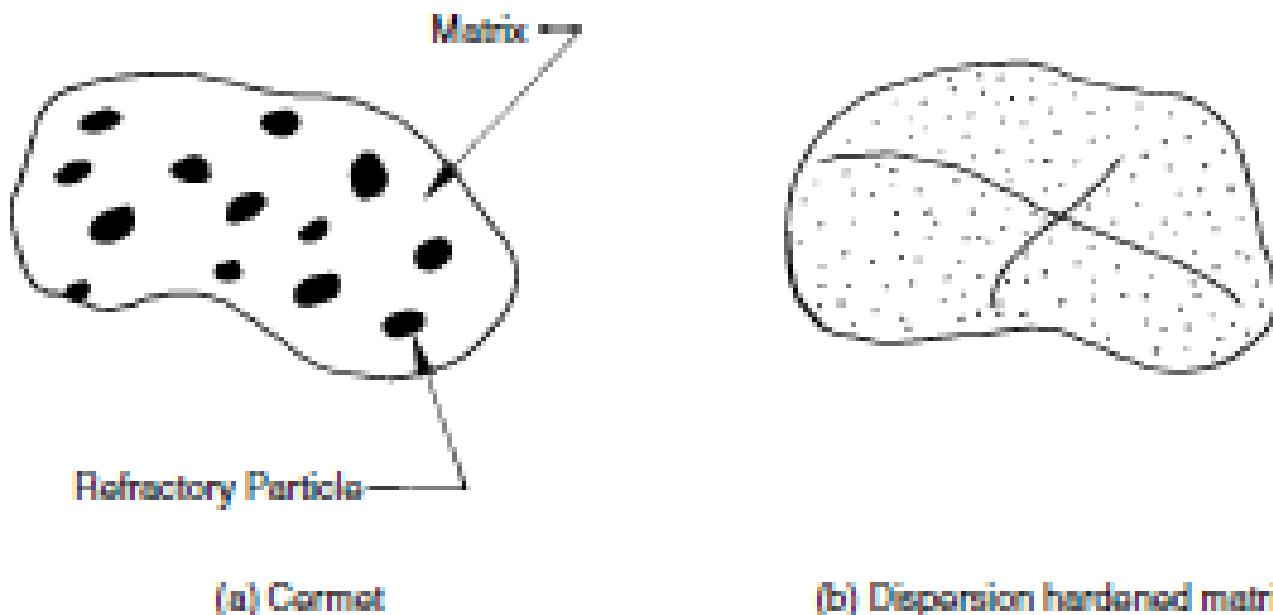


Figure 1.78 Comparison of (a) cermet and (b) dispersion-hardened alloy. Reprinted, by permission, from M. Schwartz, *Composite Materials Handbook*, 2nd ed., p. 1.32. Copyright © 1992 by McGraw-Hill.

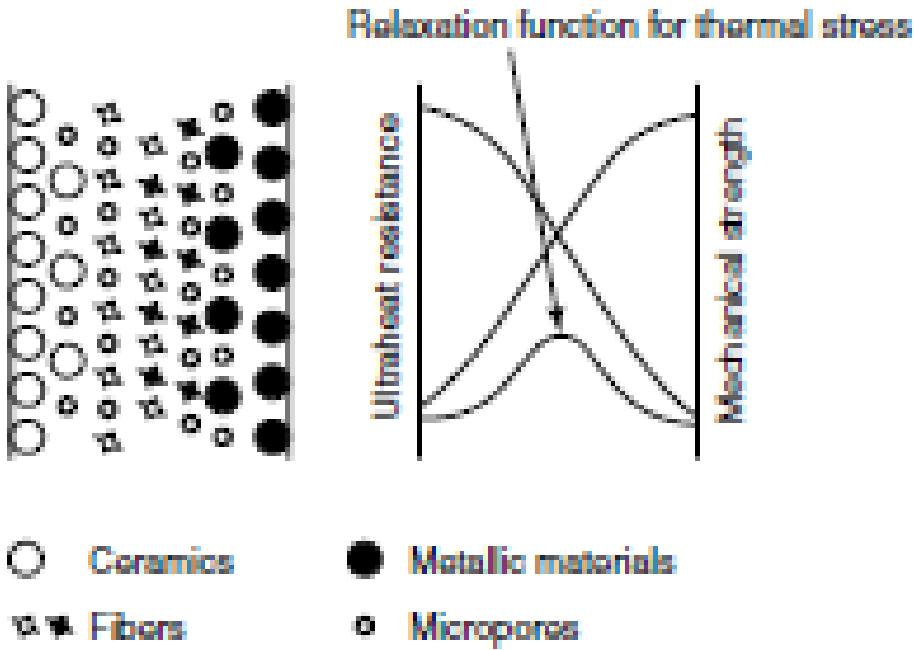


Figure I.81 Conceptual diagram of functionally graded materials (FGMs). From M. Koizumi and M. Niino, Overview of FGM research in Japan, *MRS Bulletin*, XX(1), 19 (1995). Reproduced by permission of MRS Bulletin.

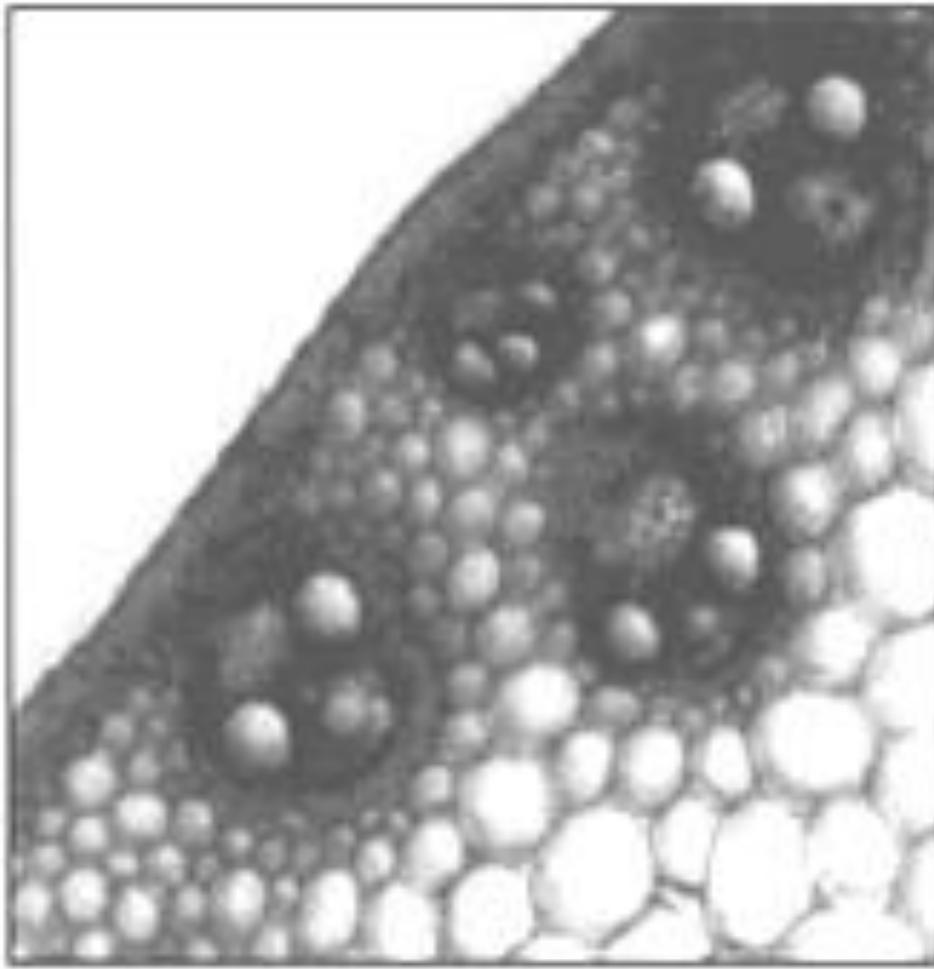


Figure 1.82 Cross-section of corn stalk exhibiting functionally graded structure. From Shigeyasu Amada, Hierarchical functionally gradient structures of bamboo, barley, and corn, *MRS Bulletin*, Vol. XX(1), 35 (1995). Reproduced by permission of MRS Bulletin.

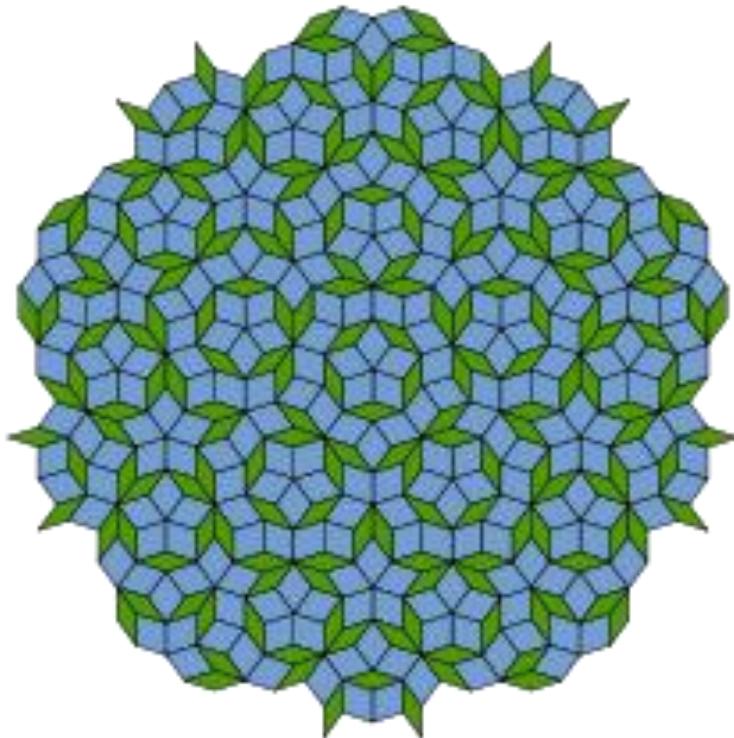
Dan Shechtman



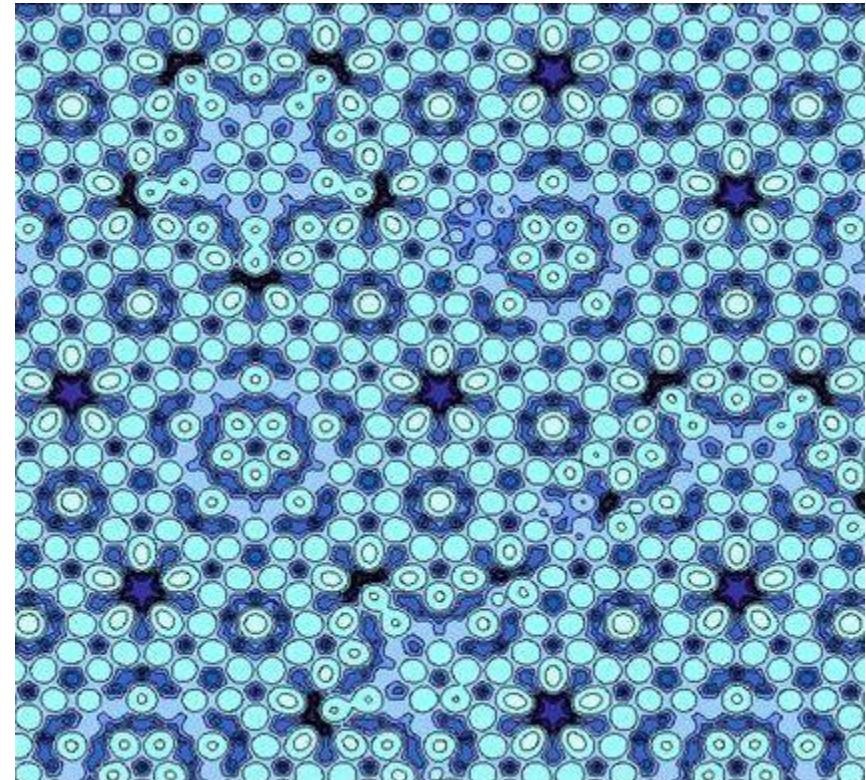
On April 8, 1982, while on sabbatical at the U.S. National Bureau of Standards in Washington, D.C., Shechtman discovered the icosahedral phase, which opened the new field of quasiperiodic crystals. He was awarded the 2011 Nobel Prize in Chemistry for "the discovery of quasicrystals". - Wikipedia

QUASI-CRYSTALS

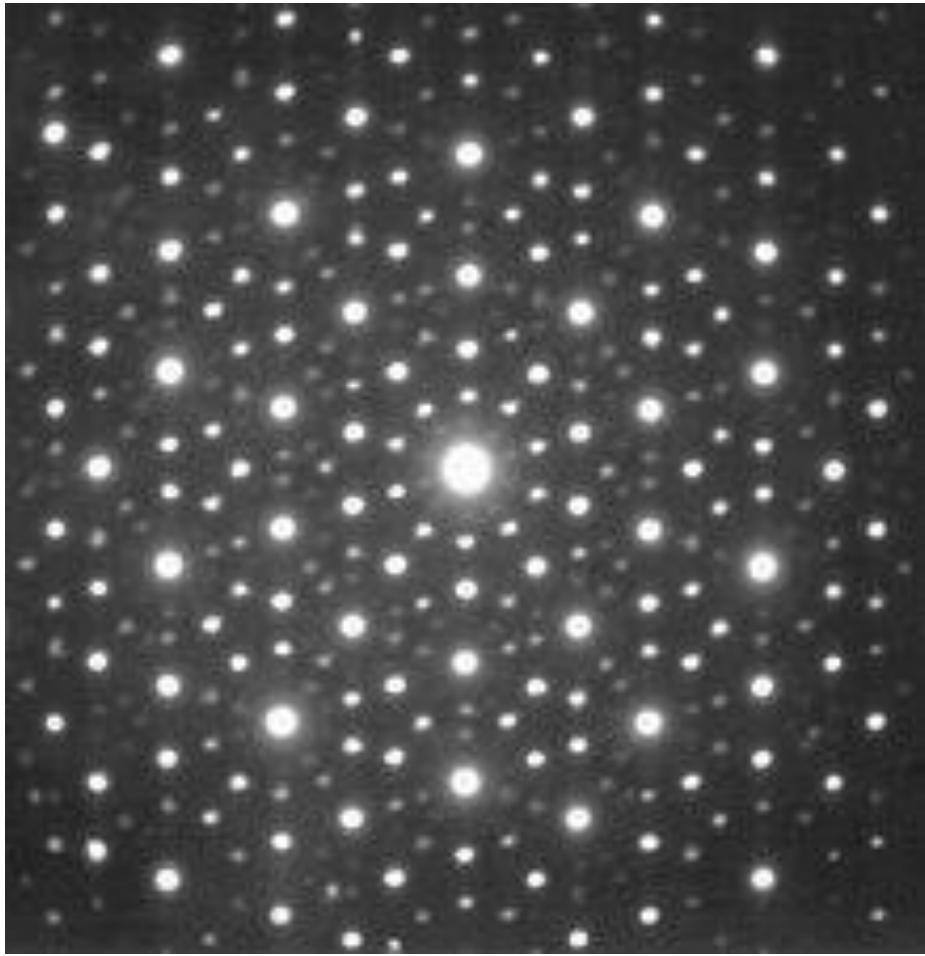
A quasiperiodic crystal, or, in short, **quasicrystal**, is a structure that is ordered but not periodic.



A Penrose tiling



Atomic model of an aluminium-palladium-manganese (Al-Pd-Mn) quasicrystal surface.



Electron diffraction pattern of an icosahedral
Ho-Mg-Zn quasicrystal

In 1992, the [International Union of Crystallography](#) altered its definition of a crystal, broadening it as a result of Shechtman's findings, reducing it to the ability to produce a clear-cut diffraction pattern and acknowledging the possibility of the ordering to be either periodic or aperiodic