CRYSTAL STRUCTURE

ORDER

BOOK 61-78 STUDY

Sit on an atom & around around

what do you see ?

short range order (Liquids, amorphous)

long range order (crystals)

disordered (gas)

WE CARE ABOUT CRYSTALS

CRYSTAL = solid material with periodic structure.

periodicity is represented by a lattice (BRAVAIS)

LATTICE = infinite set of discrete points

invariant by translation / geometrical points, not necessary atoms

(BRAVAIS LATTICES)

Sit on a lattice point and look around

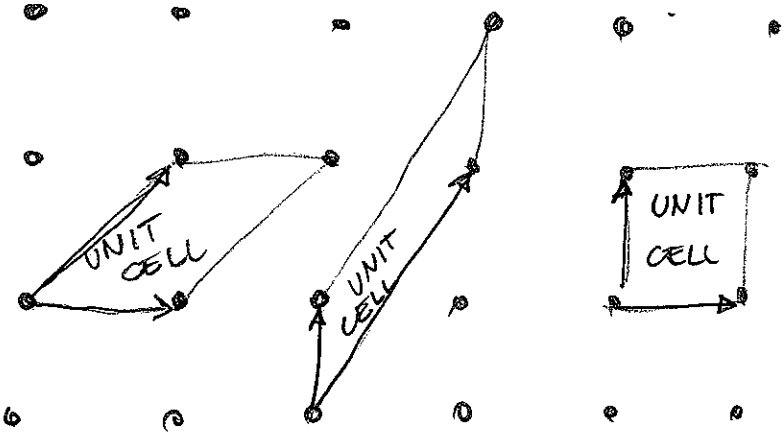
then move to another lattice point, you will see the same thing

UNIT CELL = a part of volume (surface in 2D lattice)

that is replicated for every lattice point

covers all the space once and only one

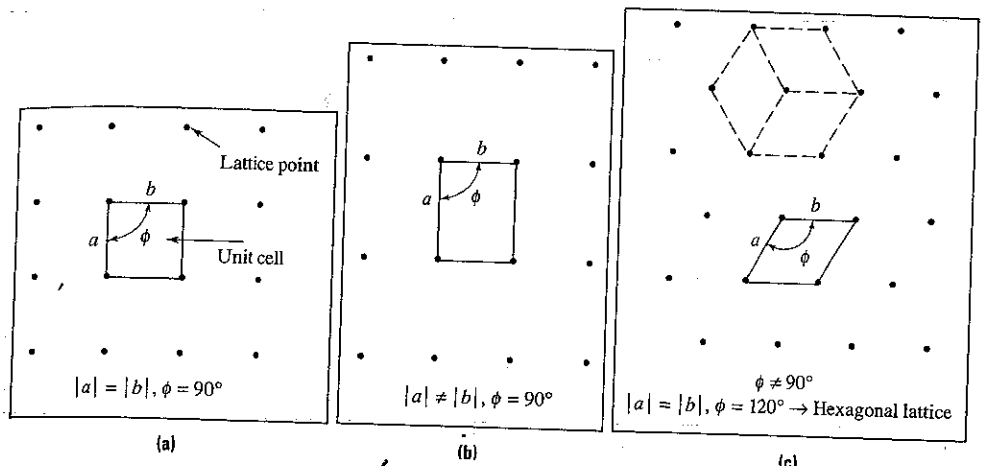
lattice points, many different unit cells



= translational vectors, $\vec{a}, \vec{b}, \vec{c}$

$|\nearrow|$ = lattice parameter

IN 2D

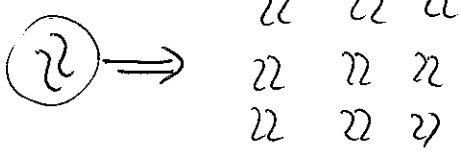


in 2D
3 possible lattices

square rectangular parallelogram, in $\phi = 120 \Rightarrow$ HEX

LATTICE = geometrical set of points needed for translations

TRANSLATION OF WHAT? OF A BASIS



LATTICE + BASIS = CRYSTAL STRUCTURE

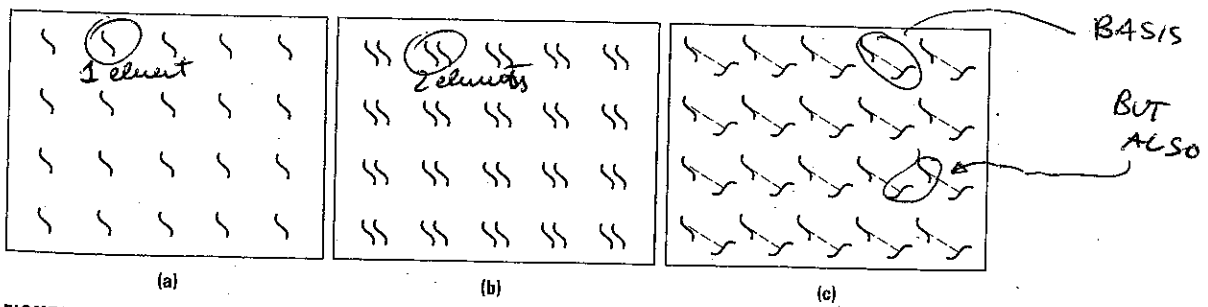


FIGURE 3.2–2 Three examples of 2-D patterns all created using the same rectangular lattice but each having a different basis: **(a)** the basis is a single character; **(b)** the basis contains a repeated character, and **(c)** the basis contains two characters with different orientations.

COORDINATION NUMBER

The points in a Bravais lattice that are closest to a given point are called its *nearest neighbors*. Because of the periodic nature of a Bravais lattice, each point has the same number of nearest neighbors. This number is thus a property of the lattice, and is referred to as the *coordination number* of the lattice. A simple cubic lattice has coordination number 6; a body-centered cubic lattice, 8; and a face-centered cubic lattice, 12. The notion of a coordination number can be extended in the obvious way to some simple arrays of points that are not Bravais lattices, provided that each point in the array has the same number of nearest neighbors.

PRIMITIVE UNIT CELL

A volume of space that, when translated through all the vectors in a Bravais lattice, just fills all of space without either overlapping itself or leaving voids is called a *primitive cell* or *primitive unit cell* of the lattice.[8] There is no unique way of choosing a primitive cell for a given Bravais lattice. Several possible choices of primitive cells for a two-dimensional Bravais lattice are illustrated in Figure 4.10.

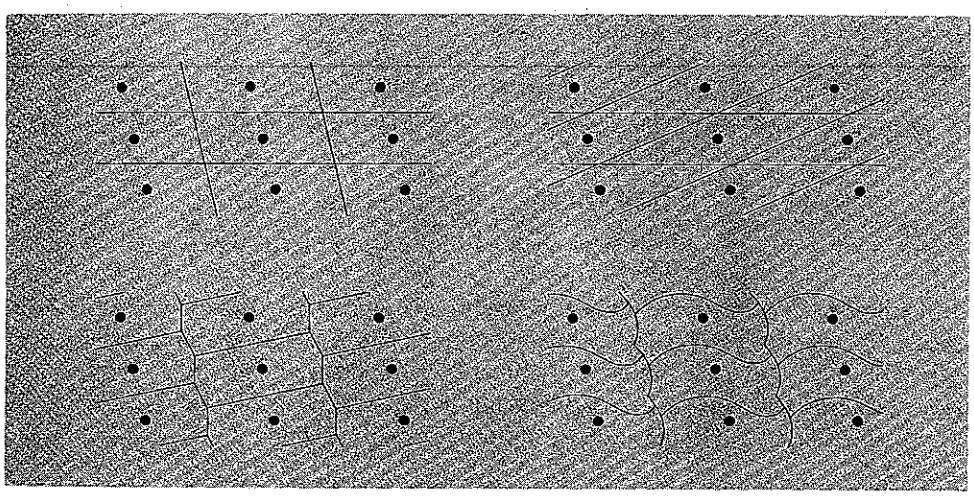


Figure 4.10
Several possible choices of primitive cell for a single two-dimensional Bravais lattice.

A primitive cell must contain precisely one lattice point (unless it is so positioned that there are points on its surface). It follows that if n is the density of points in the lattice[9] and v is the volume of the primitive cell, then $nv = 1$. Thus $v = 1/n$. Since

[8] Translations of the primitive cell may possess common surface points; the nonoverlapping proviso is only intended to prohibit overlapping regions of nonzero volume.

[9] The density n of Bravais lattice points need not, of course, be identical to the density of conduction electrons in a metal. When the possibility of confusion is present, we shall specify the two densities with different symbols.

IN 3D

14 different lattices in 7 FAMILIES
BRAVAIS

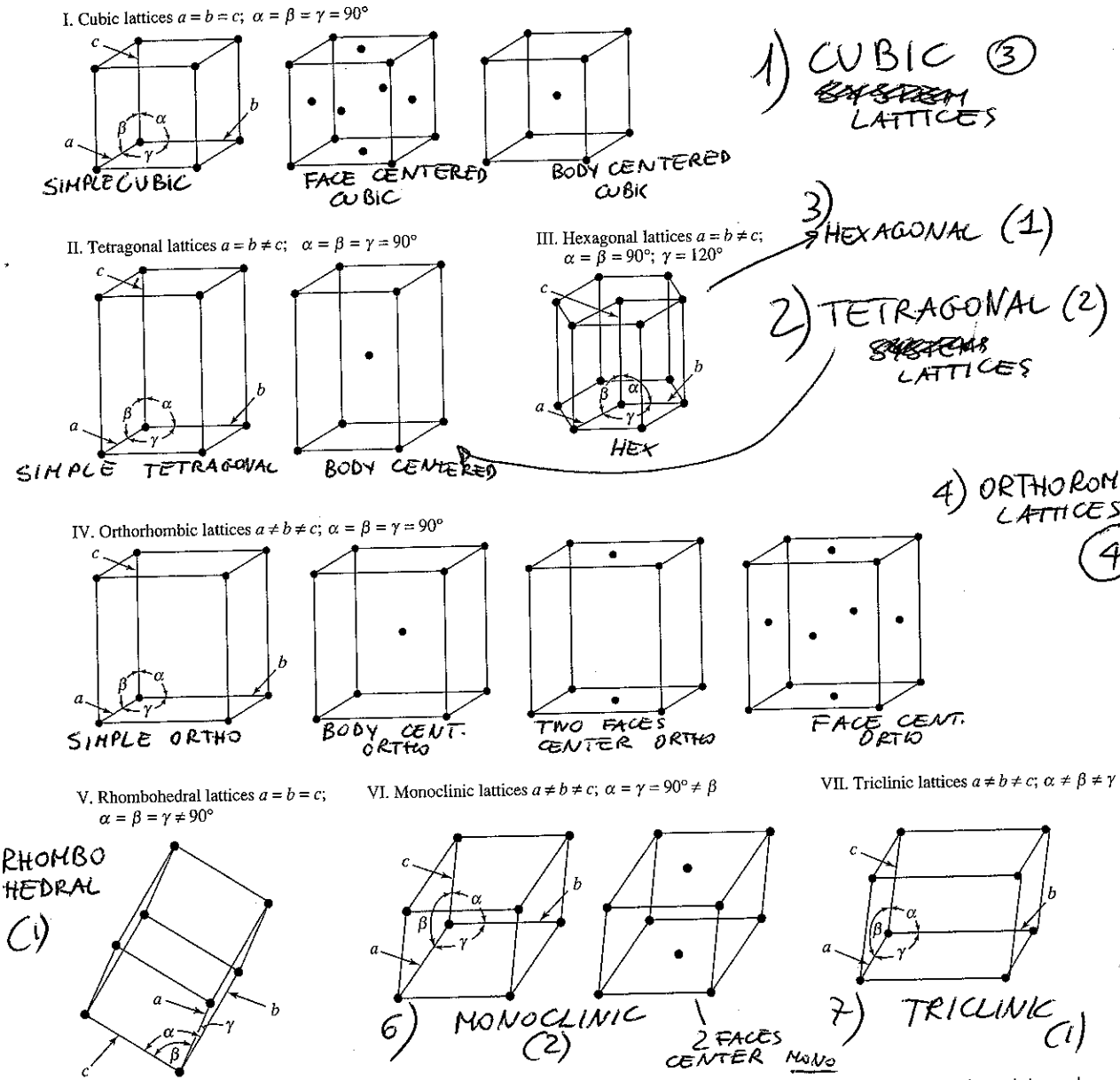


FIGURE 3.2–3 The 14 Bravais lattices grouped into the 7 lattice types. The restrictions on the lattice parameters *a*, *b*, and *c* and the angles between the edges of the unit cell α, β, and γ are listed for each unit cell.

There are 14 valid 3-D lattices...

A UNIT CELL IS THE "SMALLEST" POSSIBLE VOLUME WHICH, IF TRANSLATED, COVER ALL THE SPACE.

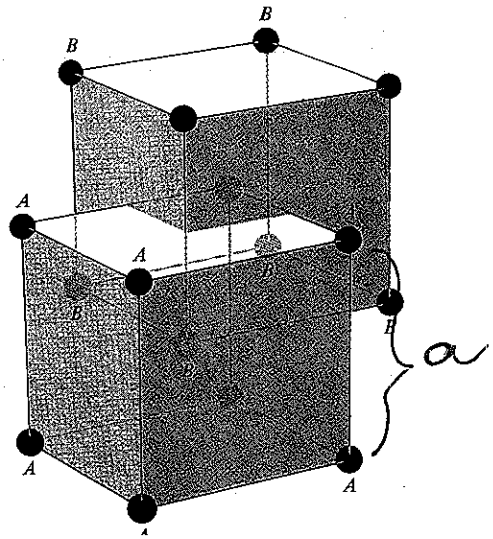
C3

SOME SYSTEMS CAN BE DESCRIBED WITH A BASIS O WITHOUT BASIS ?

BCC

EXAMPLE BCC

A few sites from a body-centered cubic Bravais lattice. Note that it can be regarded either as a simple cubic lattice formed from the points A with the points B at the cube centers, or as a simple cubic lattice formed from the points B with the points A at the cube centers. This observation establishes that it is indeed a Bravais lattice.



NO BASIS

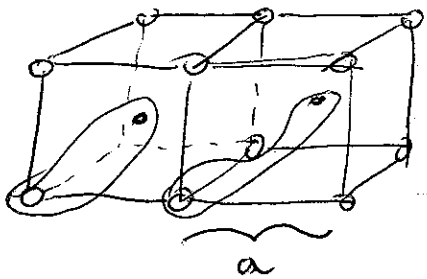
BCC = EVERY POINT IS A LATTICE POINT

a = LATTICE PARAMETER

OR WITHOUT BASIS

⇒ CUBIC LATTICE + A BASIS OF 2 POINTS

BCC OR CUBIC + BASIS



$\mathbf{0}, \quad \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$ (bcc)

ELEMENTS

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

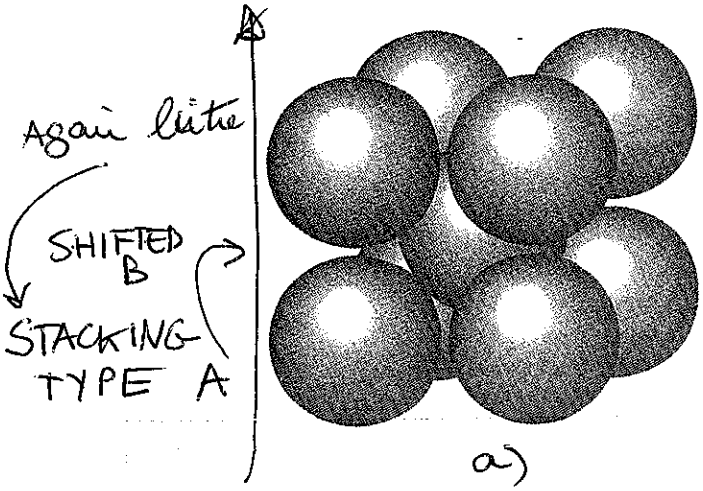
ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

TUNGSTEN

CA

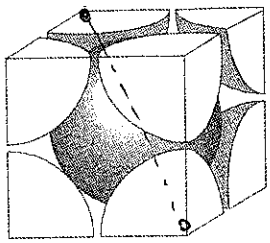
BCC

ATOMS



⇒ STACKING ABABAB

SECTION OF A UNIT CELL (CUBIC CHOICE) WITH BASIS



$a\sqrt{3}$ diagonal must FIT 2 spheres

$= 4R$

⇒

BCC WITHOUT BASIS

$a\sqrt{3} = 4R$

$\Rightarrow a = \frac{4R}{\sqrt{3}}$

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}). \tag{4.3}$$

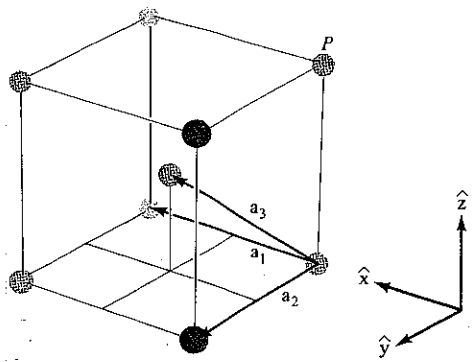


Figure 4.6
Three primitive vectors, specified in Eq. (4.3), for the body-centered cubic Bravais lattice. The lattice is formed by taking all linear combinations of the primitive vectors with integral coefficients. The point P, for example, is $P = -\mathbf{a}_1 - \mathbf{a}_2 + 2\mathbf{a}_3$.

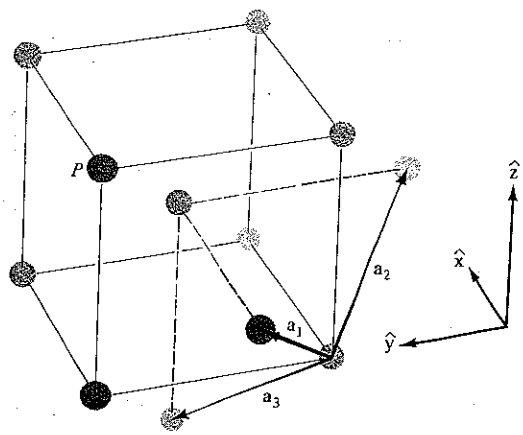


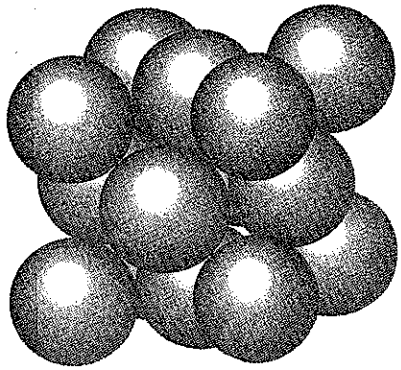
Figure 4.7
A more symmetric set of primitive vectors, specified in Eq. (4.4), for the body-centered cubic Bravais lattice. The point P, for example, has the form $P = 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

BCC WITHOUT A BASIS BUT MORE SYMMETRIC SET OF VECTOR

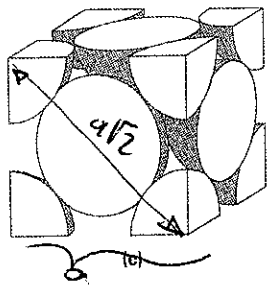
$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}). \tag{4.4}$$

C5

FCC



(b)



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

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

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \quad \text{FCC} \tag{4.5}$$

Figure 4.9
A set of primitive vectors, as given in Eq. (4.5), for the face-centered cubic Bravais lattice. The labeled points are $P = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$, $Q = 2\mathbf{a}_2$, $R = \mathbf{a}_2 + \mathbf{a}_3$, and $S = -\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

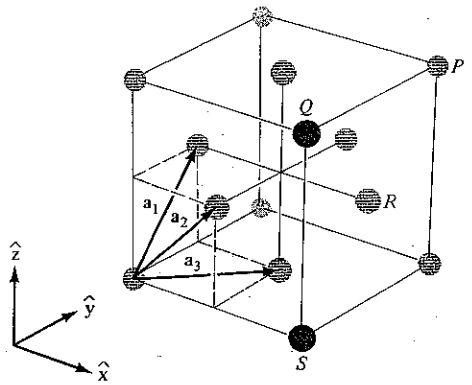


Table 4.1
ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

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

FCC LATTICE, NO BASIS
OR CUBIC LATTICE WITH BASIS OF 4!

C6

$$\mathbf{0}, \quad \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}), \quad \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}) \qquad \text{(fcc)}.$$

DIAMOND = FCC + BASIS (2)

SOME IMPORTANT EXAMPLES OF CRYSTAL STRUCTURES AND LATTICES WITH BASES

Diamond Structure

fcc, can base (1/8, 1/8, 1/8) and -( )

The diamond lattice[16] (formed by the carbon atoms in a diamond crystal) consists of two interpenetrating face-centered cubic Bravais lattices, displaced along the body diagonal of the cubic cell by one quarter the length of the diagonal. It can be regarded as a face-centered cubic lattice with the two-point basis $\mathbf{0}$ and $(a/4)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$. The coordination number is 4 (Figure 4.18). The diamond lattice is not a Bravais lattice,

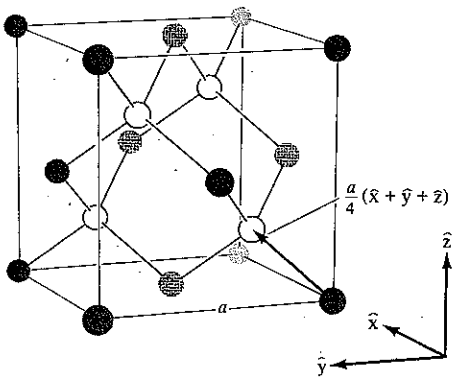


Figure 4.18
Conventional cubic cell of the diamond lattice. For clarity, sites corresponding to one of the two interpenetrating face-centered cubic lattices are unshaded. (In the zincblende structure the shaded sites are occupied by one kind of ion, and the unshaded by another.) Nearest-neighbor bonds have been drawn in. The four nearest neighbors of each point form the vertices of a regular tetrahedron.

because the environment of any point differs in orientation from the environments of its nearest neighbors. Elements crystallizing in the diamond structure are given in Table 4.3.

Table 4.3
ELEMENTS WITH THE DIAMOND CRYSTAL STRUCTURE

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

← total e density = 1.05×10^{24} e⁻/cc

Hexagonal Close-Packed Structure

Though not a Bravais lattice, the *hexagonal close-packed* (hcp) structure ranks in importance with the body-centered cubic and face-centered cubic Bravais lattices; about 30 elements crystallize in the hexagonal close-packed form (Table 4.4).

[16] We use the word "lattice," without qualifications, to refer either to a Bravais lattice or a lattice with a basis.

C6b

HEX

IS A BRAVAIS LATTICE

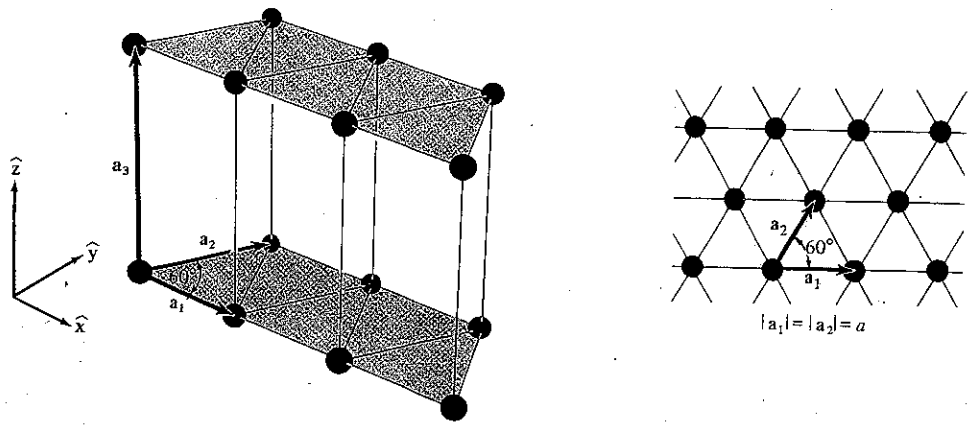


Figure 4.19
The simple hexagonal Bravais lattice. Two-dimensional triangular nets (shown in inset) are stacked directly above one another, a distance c apart.

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = \frac{a}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}a}{2}\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}.$$

PRIMITIVE VECTORS

HCP IS NOT A BRAVAIS LATTICE

HEXAGONAL CLOSED PACKED

HCP = HEX + BASIS(2)

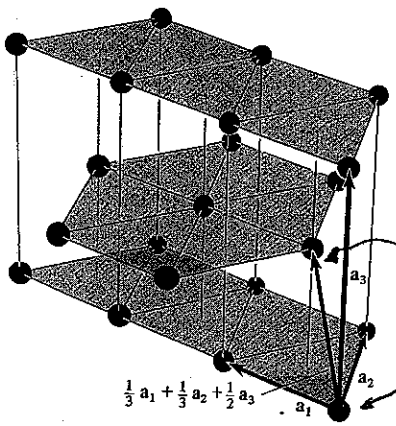
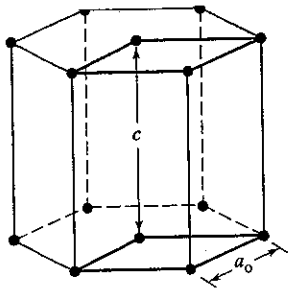


Figure 4.20
The hexagonal close-packed crystal structure. It can be viewed as two interpenetrating simple hexagonal Bravais lattices, displaced vertically by a distance $c/2$ along the common c-axis, and displaced horizontally so that the points of one lie directly above the centers of the triangles formed by the points of the other.

HCP = HEX + BASIS

C7

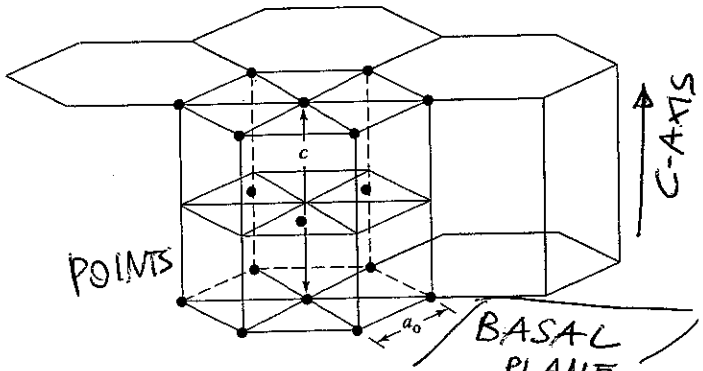
HCP



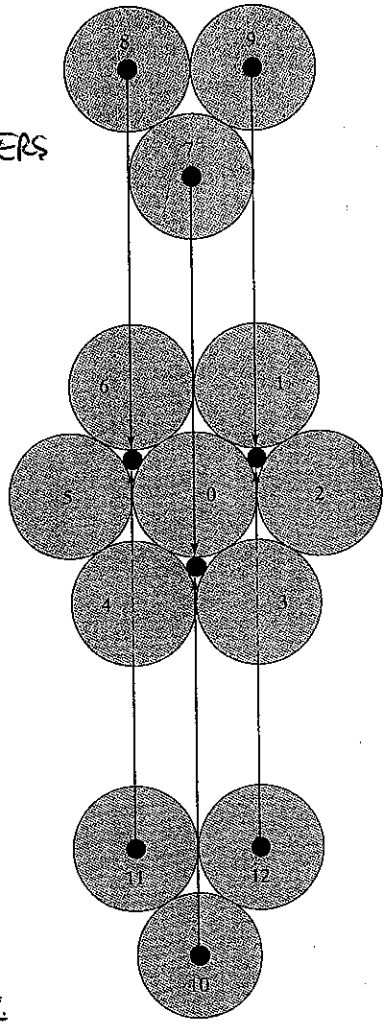
(a)

UNIT CELL

NEED 2 PARAMETERS

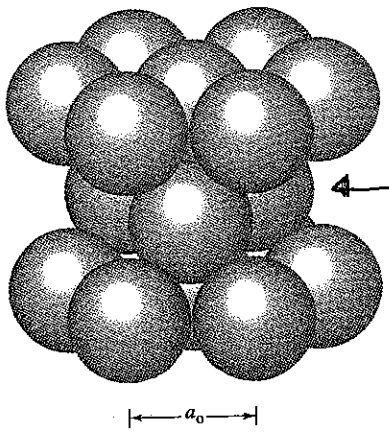


(b)



(d)

STACKING



(c)

ATOMS

WITHOUT THIS IS NORMAL HEXAGONAL

Table 4.4
ELEMENTS WITH THE HEXAGONAL CLOSE-PACKED CRYSTAL STRUCTURE

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

IDEAL (WITH SPHERES)

$$c = \left(\frac{4}{\sqrt{6}}\right)a_0 = 1.633a_0 = 3.266r$$

VOLUME

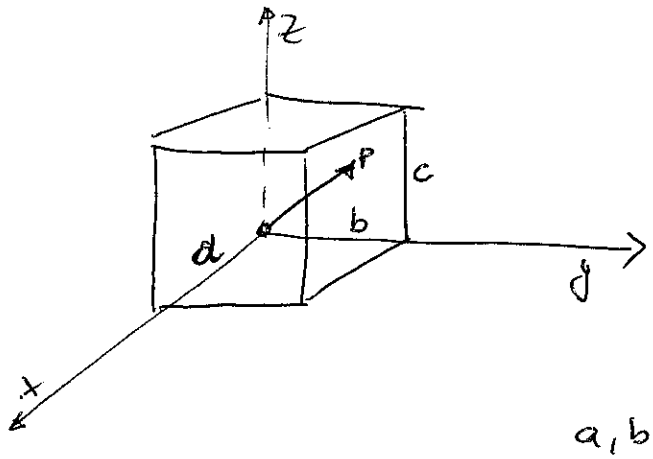
$$V_{uc}(\text{large HCP}) = \left(\frac{3\sqrt{3}}{2}\right)a_0^2 c$$

C 8

MILLER INDICES

- CUBIC, TETRAGONAL, ORTHORHOMBIC

for all the systems with angles $\alpha=\beta=\gamma=90$

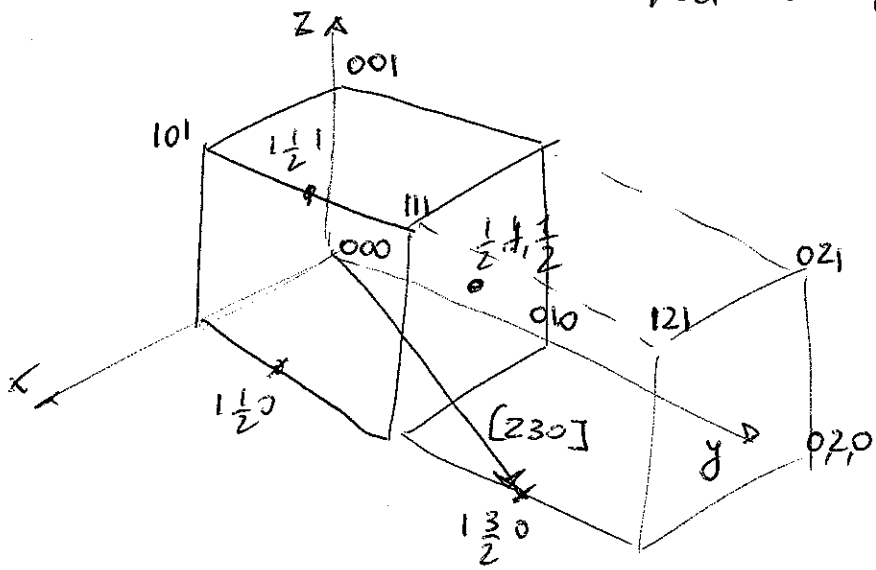


RIGHT HAND CARTESIAN SYSTEM

TAKE "RECTANGULOID" UNIT CELL

a, b, c in meters [may be Å OR nm]

(h, k, l) = fractions of positions of P with respect to (a, b, c).



POINTS

FRACTIONAL

negative put a $-$ on the top

DIRECTIONS

put numbers in (h, k, l) and get

MAXIMUM COMMON DENOMINATOR $\Rightarrow$ DIVIDE

MINIMUM COMMON MULTIPLIER $\Rightarrow$ MULTIPLY

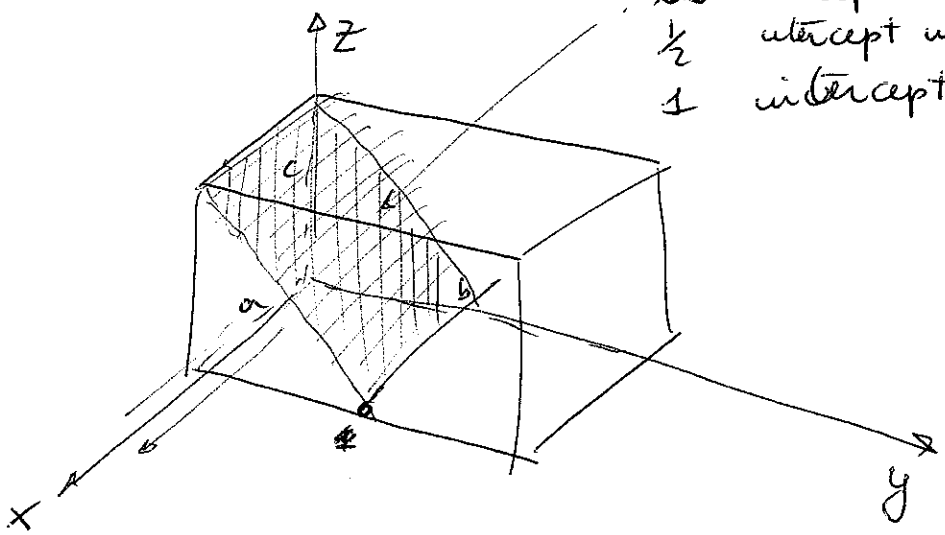
$(1\ \frac{3}{2}\ 0) \Rightarrow [2\ 3\ 0]$

$(2\ 2\ 0) \Rightarrow [1\ 1\ 0]$

$\Longrightarrow$ MILLER INDICES

PLANES

1) MAKE COORDINATES



∞ intercept in $\hat{x}$
$\frac{1}{2}$ intercept in $\hat{y}$
1 intercept in $\hat{z}$

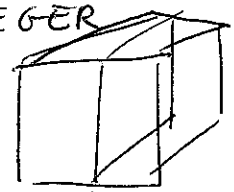
2) identify intercepts in $(h\ k\ \ell)$ notation (fractional), in the $\hat{x}, \hat{y}, \hat{z}$ axis

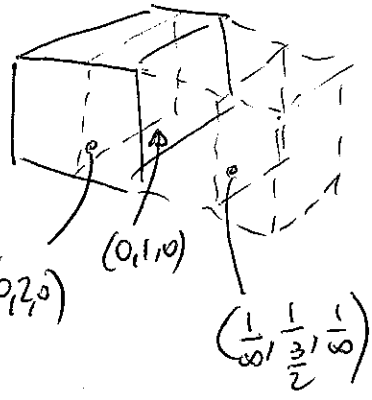
3) take reciprocal

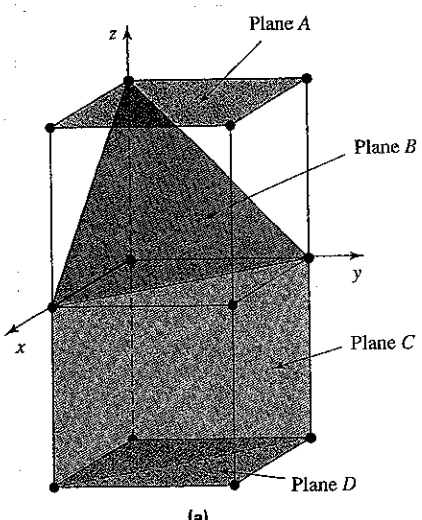
$\left(\frac{1}{h}, \frac{1}{k}, \frac{1}{\ell}\right) \rightarrow \left(\frac{1}{\infty}, \frac{1}{1/2}, \frac{1}{1}\right) \rightarrow (0, 2, 1)$

→ plot (−) on top of negative

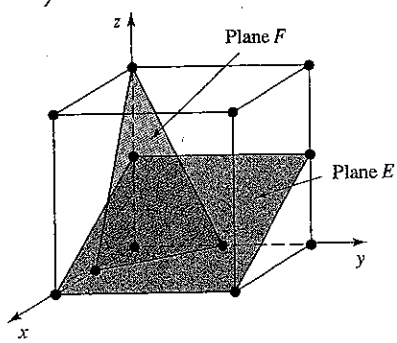
4) clear fractions but DO NOT REDUCE AT LOWER INTEGER







(a)



Plane	Intercepts	Indices
A	∞, ∞, 1	(0 0 1)
B	1, 1, 1	(1 1 1)
C	1, 1, ∞	(1 1 0)
D	∞, ∞, –1	(0 0 $\bar{1}$)
E	1, ∞, 1/2	(1 0 2)
F	1/2, 1/2, 1	(2 2 1)

(b)

C10

DENSITY, PACKING FACTORS OF CRYST.

MUST COUNT ONLY LATTICE POINTS (BRAVAIS) NOT ATOM
NECESSARY (UNLESS BASIS = 1 element)

BOOK
1) PICK 1 DIRECTION, PUT IN MILLER NOTATION
2) COUNT # OF EQUIVALENT LATTICE POINTS
3) DIVIDE BY THEIR DISTANCE

$$\Rightarrow \rho_L = \frac{\#\text{ of LATTICE POINTS ALONG DIRECTION IN UNIT CELL}}{\text{LENGTH OF LINE CONTAINED IN ONE UNIT CELL}} \quad \left[\frac{1}{m}\right]$$

EQUIVALENT NOTATION, BUT EASIER! (STEFANO'S)

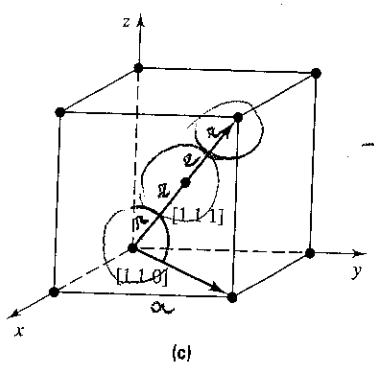
1) PICK 1 DIRECTION FROM ORIGIN (1 POINT 000)
2) MEASURE DISTANCE WITH 1ST EQUIVALENT POINT OF ORIGIN = d

$$\Rightarrow \rho_L(\text{DIRECTION}) = \frac{1}{d_{hkl}(\text{DIRECTION})}$$

put DIST IN RADII OF SPHERES

EXAMPLE 3.5.1 (79)

BCC



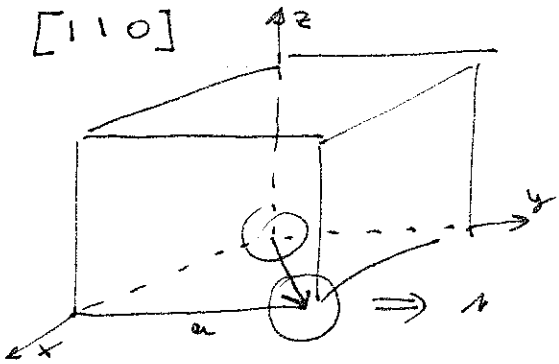
along [1 1 1]

$a\sqrt{3} = 4r$ (relation $r \leftrightarrow$ lattice parameter for BCC)

start from (0,0,0)
go along [1 1 1] $\Rightarrow$ meet $\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$
at position $\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ distance
$= 2r \Rightarrow \rho_L([1\,1\,1]) = \frac{1}{2r}$ //

C11

ALONG [1 1 0]



$a\sqrt{3} = 4r$

$\Rightarrow a = 4r/\sqrt{3}$

go along [110]

$\Rightarrow$ meet point (1,1,0) @ distance $a\sqrt{2}$

$$\Rightarrow \rho_L([110]) = \frac{1}{a\sqrt{2}} = \frac{\sqrt{3}}{r4\sqrt{2}} \leq \frac{0.3}{r}$$

SYMMETRY

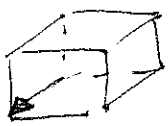
$$\rho_L[110] = \rho_L[101] = \rho_L[011] \simeq \frac{0.3}{r}$$

$$\rho_L[111] = \frac{0.5}{r}$$

$$\rho_L[100] = \rho_L[010] = \rho_L[001] \simeq \frac{0.43}{r}$$

CLOSE PACKING DIRECTION

ALONG [1 0 0]



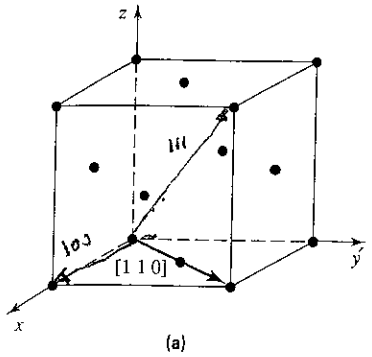
go along [100]

meet point (1,0,0) @ a

$$\rho_L([100]) = \frac{1}{a} = \frac{\sqrt{3}}{4r} \simeq 0.43\frac{}{r}$$

CLOSE PACKING DIRECTION IS THE DIRECTION WHERE EQUIVALENT POINTS ARE CLOSER!!! (HIGHEST ρ_L)

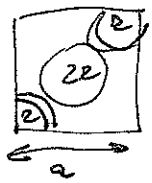
FCC



(a)

RATIO $a \leftrightarrow r$ for FCC

FACE



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

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

along [111] find $(1,1,1)$ @ $a\sqrt{3} \Rightarrow$

$\rho_L[111] = \frac{1}{a\sqrt{3}} = \frac{\sqrt{2}}{4r\sqrt{3}} \simeq \frac{0.2}{r}$

along [110] or [101] or [011]

find $(\frac{1}{2}, \frac{1}{2}, 0)$ @ $\frac{a\sqrt{2}}{2} = \frac{a}{\sqrt{2}} \Rightarrow$ $\rho_L[111] = \frac{\sqrt{2}}{a\sqrt{2}} = \frac{\sqrt{2}\sqrt{2}}{4r} = \frac{1}{2r} = \frac{0.5}{r}$

along [100] or [010] or [001]

find $(1,0,0)$ @ $a \Rightarrow \rho_L[100] = \frac{1}{a} = \frac{\sqrt{2}}{4r} \simeq \frac{0.35}{r}$

CLOSE-PACKING DIRECTION FOR FCC = [110]

the cubic

C13

PLANAR DENSITY

PLANAR DENSITY IS THE DENSITY OF POINTS PER UNIT AREA

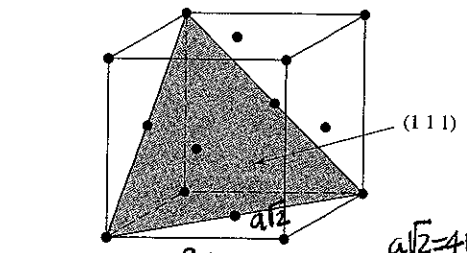
$$\rho_P(\text{PLANE}) = \frac{\#\text{ OF POINTS LATTICE}}{\text{AREA OF THE SURFACE CONSIDERED}}$$

(PICK SURFACE INSIDE UNIT CELL FOR SIMPLICITY BUT NOT NECESSARY!!)

AS FOR LINEAR DENSITY, SUBSTITUTE POINTS WITH SPHERES OF RADIUS R SO YOU CAN COMPARE DIFFERENT STRUCTURES (AND YOU ARE READY TO RUN IF THE BASIS IS MONOATOMIC !!)

FCC

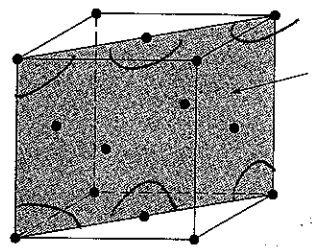
EX 3.5-2



ALONG [111] (a)

$a\sqrt{2} = 4r$

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



$\rho_P[110] = \frac{2}{a\sqrt{2}\cdot a} =$

$\frac{2}{a^2\sqrt{2}} = \frac{2}{\sqrt{2}\,16r^2/2}$

$\Rightarrow \boxed{\rho_P(110) = \frac{1}{4\sqrt{2}\,r^2}}$ NICE BOX

$\rho_P(100) = \rho_P(200) = \frac{1}{8r^2}$

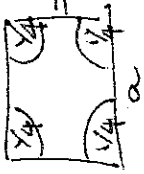
NICE BOX :)

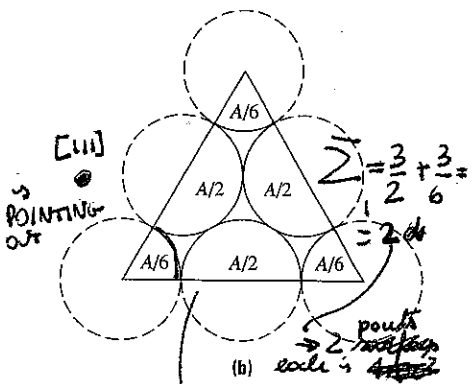
$\rightarrow \boxed{\rho_P[111] = \frac{1}{r^2 2\sqrt{3}}}$

$\rho_P(100) = \frac{1}{a^2} = \frac{2}{16r^2} = \frac{1}{8r^2}$

$\Rightarrow 4\cdot\frac{1}{4} = 1$

$\rho_P[110] =$





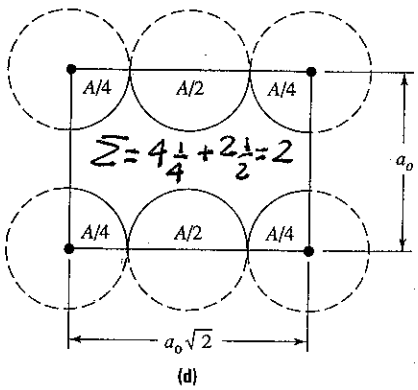


FIGURE 3.5–2 **(a)** The portion of the (1 1 1) plane contained within a single FCC unit cell is sketched in 3-D; **(b)** the same plane sketched in 2-D; **(c)** the portion of the (1 1 0) plane contained within a single FCC unit cell is sketched in 3-D; **(d)** the same plane sketched in 2-D.

$\rho_P[111] = \frac{2}{\text{area}} = \frac{1}{2r^2\sqrt{3}}$

CLOSE PACKED

area $= \frac{1}{2}\, a\sqrt{2}\, \frac{a\sqrt{3}}{\sqrt{2}} \Rightarrow$

$A = a\sqrt{2}\,\frac{a\sqrt{3}}{\sqrt{2}}\,\frac{1}{2} = \frac{a^2\sqrt{3}}{2} \Rightarrow \rho_P = \frac{2}{\frac{a^2\sqrt{3}}{2}} = \frac{4}{a^2\sqrt{3}} = \frac{4}{\frac{16r^2}{2}\sqrt{3}} = \frac{1}{2\sqrt{3}r^2}$

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

CH

HIGHEST DENSITY PLANE

⇒ FOR FCC ρ_P MAX IS $\rho_P(111) = \frac{1}{2\sqrt{3}R^2}$ MAX OF EVERY THING

⇒ such $\rho_P = \frac{1}{2\sqrt{3}R^2}$ is called CLOSE-PACKED PLANE → in a system with HIGHEST DENSITY PLANE IS = to CLOSE PACKED → IT IS CALLED CLOSE PACKED

THEN

BCC $\rho_P^{BCC}(110) = \frac{3}{8R^2\sqrt{2}} \simeq 92\%$ of $\rho_P^{FCC}(111)$

HIGHEST DENSITY PLANE → BCC IS NOT CLOSE-PACKED

FOR HOME $\rho_P^{BCC}(100)$, $\rho_P^{BCC}(111)$, $\rho_P^{BCC}(210)$? FAST ☹

$\rho_P^{FCC}(111)$ is THE HIGHEST DENSITY PLAUE

TABLE 3.5–1 The close-packed directions and highest-density planes in the BCC, FCC, and HCP crystal structures.

Crystal structure	Close-packed directions	Highest-density planes	Are the highest-density planes close-packed?
BCC	⟨1 1 1⟩	{1 1 0}	No
FCC	⟨1 1 0⟩	{1 1 1}	Yes
HCP	a_1	Basal	Yes

CLOSE PACKED IF $\rho_P^{MAX} = \frac{1}{2\sqrt{3}R^2}$

BCC IS NOT C.P.

FCC is C.P. for plane (111)

→ HCP = HEX + BASIS is C.P. on the basal plane

SEE LATER

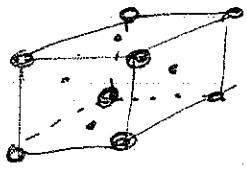
CIS

VOLUMETRIC DENSITY:

$\rho_V = \frac{\#\text{ of LATTICE POINT}}{\text{UNIT VOLUME}}$ → 1) put POINTS as spherical atoms
2) count them in UNIT CELL (TAKE an easy one)
3) $\rho_V = \#/\text{Volume}$

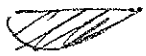
FCC

for simplicity we take CUBIC UNIT CELL



HAVE 8 corners spheres with 1/8 volume each

HAVE 6 face spheres with 1/2 volume



$\Rightarrow \#\text{atoms} = 8*\frac{1}{8} + 6*\frac{1}{2} = 4$

$V_{cube} = a^3 \Rightarrow a = \frac{4r}{\sqrt{2}} \Rightarrow \rho_V = \frac{4}{4^3 r^3 \sqrt{2}^3} =$

$$\rho_V^{FCC} = \frac{1}{4\sqrt{2}r^3}$$

HCP is same $\rho_V^{HCP} = \frac{1}{4\sqrt{2}r^3}$ if $c/a = 1.6$ theoretical one

EXERCISE ρ_V^{BCC} ?

HCP & FCC were both CLOSED PACKED STRUCTURE

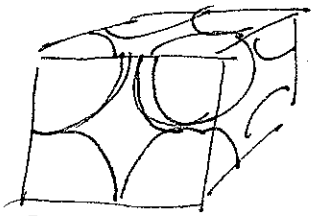
HCP = HEX CLOSED PACKED

ATOMIC PACKING FACTOR

measures the empty volume of the cell!!

APF ↑ empty volume ↓

= occupied fraction of volume



SIMPLE CUBIC

$$APF \equiv \frac{\text{Volume atoms (if spherical)}}{\text{Volume cell}}$$

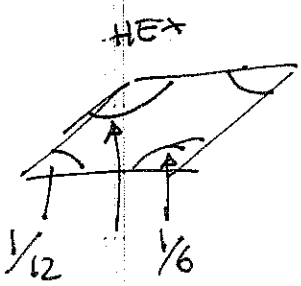
$\Rightarrow$

each sphere is $\boxed{\frac{4}{3}\pi r^3}$

	ATOMS/CUBIC CELL	$a \leftrightarrow r$ relation	APF
SIMPLE CUBIC	$8*\frac{1}{8} = 1$	$a = 2r$	$1*\frac{4}{3}\pi r^3 / 8r^3 = 0.52$
BCC	$8*\frac{1}{8} + 1 = 2$	$a = \frac{4r}{\sqrt{3}}$	0.68
FCC	$8*\frac{1}{8} + 6*\frac{1}{2} = 4$	$a = \frac{4r}{\sqrt{2}}$	0.74
HCP (ideal $c/a = 1.6$)	$4*\frac{1}{6} + 4*\frac{1}{12} + 1 = 2$	$c = 1.633\,a = 3.266\,r$ IDEAL	0.74

MOST DENSE!!

HCP = HEX + BASIS (2)
EXTRA ATOM IS IN CENTER



$$c = \left(\frac{4}{\sqrt{6}}\right)a = 1.633$$

CLOSE PACKED STRUCTURES

FCC & HCP are the most DENSE STRUCTURES

↓ LATTICE — ↓ HEX + BASIS LATTICE

they are very SIMILAR

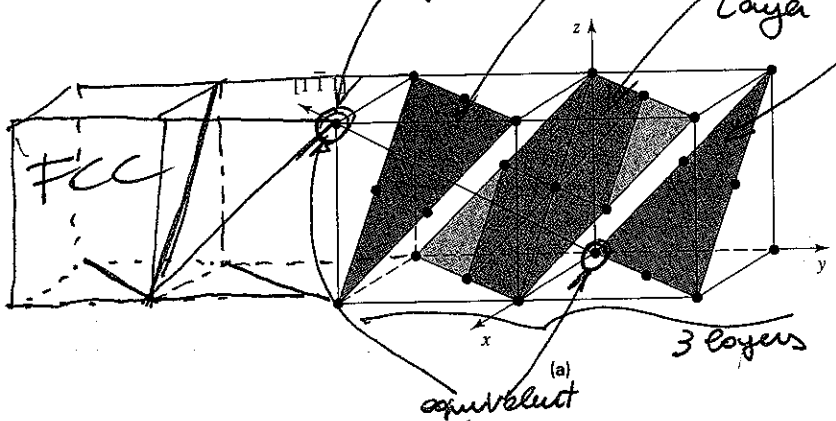
FCC in [111] direction is an HEX LATTICE + BASIS (3)

HCP in AXIS direction is an HEX LATTICE + BASIS (2)

[111]

FCC

same as FIRST layer — third layer — Second Layer — 1st Layer

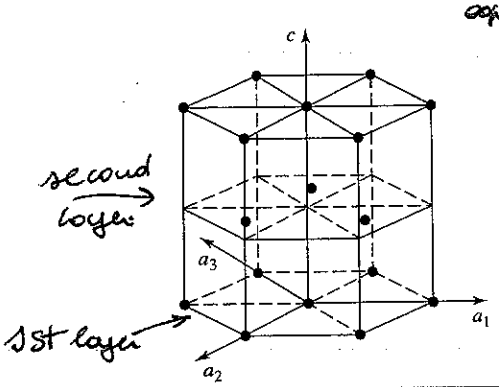


3 layers ABC

equivalent

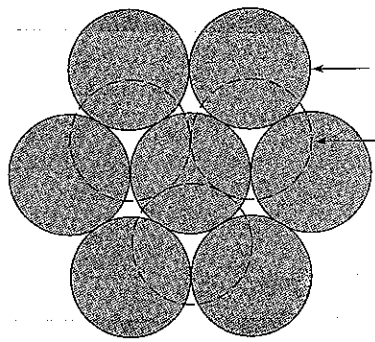
(a)

HCP

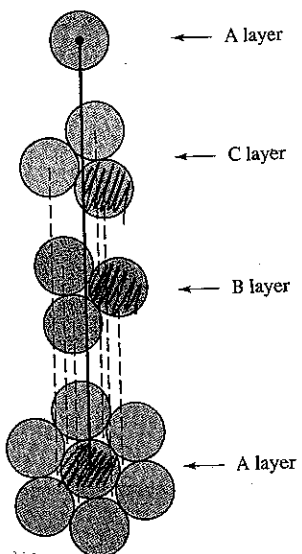


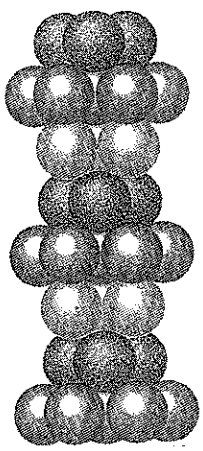
second layer →

1st layer →



FCC is HEX + BASIS OF 3

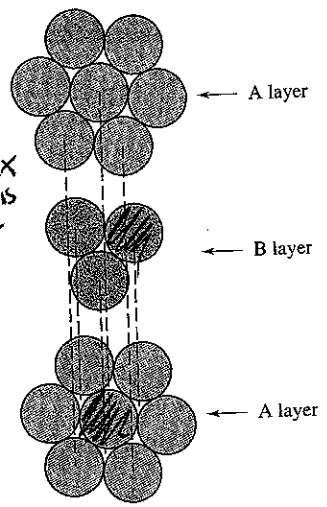


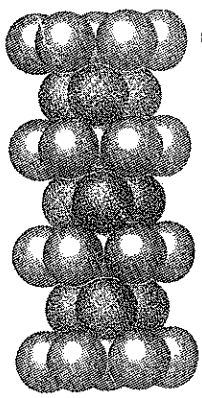


Cubic close packing

HCP is HEX + BASIS OF 2

C AXIS





Hexagonal close packing

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INTERSTITIAL POSITION → WHY? TO SQUEEZE SOMETHING ELSE INSIDE

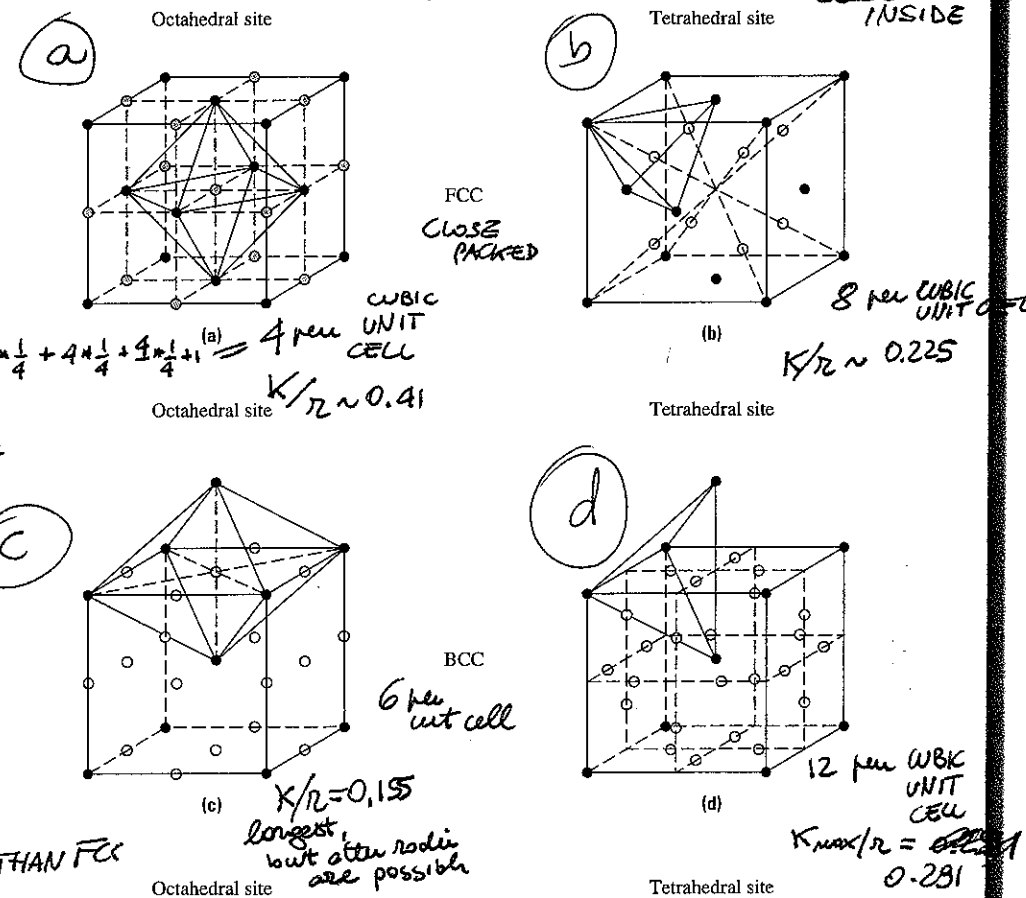

FIGURE 3.6–1
The locations of the interstitial sites in the common crystal structures: **(a)** octahedral sites in FCC, **(b)** tetrahedral sites in FCC, **(c)** octahedral sites in BCC, **(d)** tetrahedral sites in BCC, **(e)** octahedral sites in HCP, and **(f)** tetrahedral sites in HCP.

$4 \times \frac{1}{4} + 4 \times \frac{1}{4} + 4 \times \frac{1}{4} + 1 = 4$ per cubic unit cell

X = max radius of an INTRUDER

BCC is NOT C.P.
⇒ SOLUTION IS NOT EQUIDISTANT
⇒ BCC IS OPEN STRUCTURE
INTRUDERS CAN GET IN/OUT EASIER THAN FCC

longest, but other radii are possible

Because both closed packed

3.6.2 Interstices in the BCC Structure

Like the FCC structure, the BCC structure also contains both octahedral and tetrahedral sites. As shown in Figure 3.6–1c, the octahedral sites are located in the center of each face and the center of each edge, giving a total of six sites per unit cell. The diameter of the octahedral site cannot be determined by examination of the face diagonal. The BCC structure is not a close-packed structure, and the atoms that surround the interstitial site are not all equidistant neighbors. When the largest possible atom occupies the octahedral position, the atoms touch only along ⟨1 0 0⟩ as measured from one central atom to

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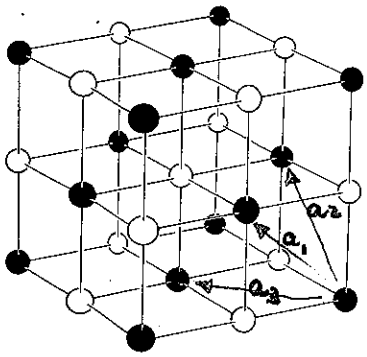
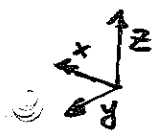
CRYSTALS WITH 2 ATOMS/CELL

SODIUM CHLORIDE STRUCT. Prototype NaCl Rocksalt

IONIC





- BLACK ATOMS FORM FCC LATTICE
- WHITE ATOMS ARE SECOND ATOM IN BASIS

OR VICEVERSA

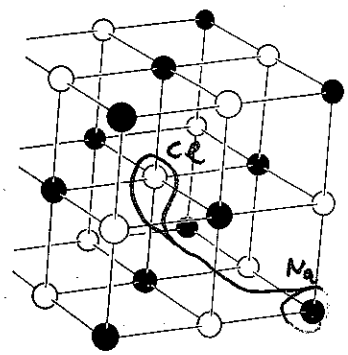
SODIUM CHLORIDE STRUCTURE =

FCC + BASIS(2)

⇓

FCC ⇒

$$a_1 = \frac{a}{2}(\hat{y}+\hat{z})$$
$$a_2 = \frac{a}{2}(\hat{z}+\hat{x})$$
$$a_3 = \frac{a}{2}(\hat{x}+\hat{y})$$



(0,0,0) Na

$\frac{a}{2}(1,1,1)$ Cl

↓

BUT EVERY COUPLE OF ● & ○ will work

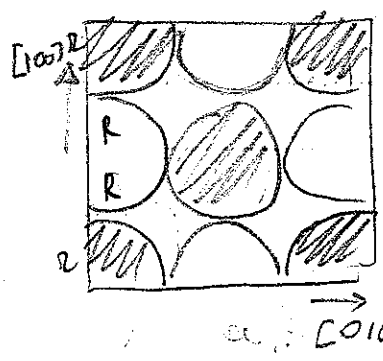
SEE PHOTOCOPY FOR EXAMPLE

- OR YOU CAN CONSIDER AS 2 INTERPENETRATING FCC LATTICES

a ⇔ 2r

ALONG [100] DIR

FACE



$\Rightarrow \boxed{2(2r+R) = a}$

The Sodium Chloride Structure

We are forced to describe the hexagonal close-packed and diamond lattices as lattices with bases by the intrinsic geometrical arrangement of the lattice points. A lattice with a basis is also necessary, however, in describing crystal structures in which the atoms or ions are located only at the points of a Bravais lattice, but in which the crystal structure nevertheless lacks the full translational symmetry of the Bravais lattice because more than one kind of atom or ion is present. For example, sodium chloride (Figure 4.24) consists of equal numbers of sodium and chlorine ions placed at alternate points of a simple cubic lattice, in such a way that each ion has six of the other kind of ions as its nearest neighbors.[17] This structure can be described as a face-centered cubic Bravais lattice with a basis consisting of a sodium ion at **0** and a chlorine ion at the center of the conventional cubic cell, $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

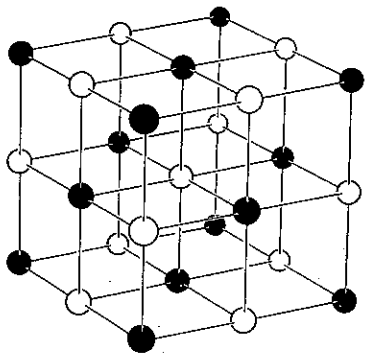


Figure 4.24
The sodium chloride structure. One type of ion is represented by black balls, the other type by white. The black and white balls form interpenetrating fcc lattices.

NACl
interpenetrating FCC

FCC + BASIS $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$ Na
0 Cl

Table 4.5
SOME COMPOUNDS WITH THE SODIUM CHLORIDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
LiF	4.02	RbF	5.64	CaS	5.69
LiCl	5.13	RbCl	6.58	CaSe	5.91
LiBr	5.50	RbBr	6.85	CaTe	6.34
LiI	6.00	RbI	7.34	SrO	5.16
NaF	4.62	CsF	6.01	SrS	6.02
NaCl	5.64	AgF	4.92	SrSe	6.23
NaBr	5.97	AgCl	5.55	SrTe	6.47
NaI	6.47	AgBr	5.77	BaO	5.52
KF	5.35	MgO	4.21	BaS	6.39
KCl	6.29	MgS	5.20	BaSe	6.60
KBr	6.60	MgSe	5.45	BaTe	6.99
KI	7.07	CaO	4.81		

The Cesium Chloride Structure

Similarly, cesium chloride (Figure 4.25) consists of equal numbers of cesium and chlorine ions, placed at the points of a body-centered cubic lattice so that each ion

[17] For examples see Table 4.5.

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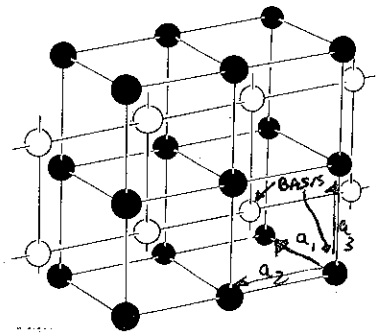
CESIUM CHLORIDE STRUCTURE prototype CsCl



IONIC

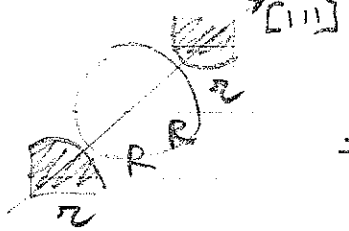
2 INTERPENETRATING CUBIC

CSCL = CUBIC + BASIS (2)

$a_1 = a\hat{x}$ $a_2 = a\hat{y}$ $a_3 = a\hat{z}$

↳ $(0,0,0)$, $\frac{a}{2}(1,1,1)$

a ⇔ r relation, along direction [1 1 1]



$\Rightarrow$ $a\sqrt{3} = 2(r+R)$

CAN BE SEEN AS BCC WITH BLACK/WHITE ALTERNATING ATOMS

has eight of the other kind as its nearest neighbors.[18] The translational symmetry of this structure is that of the simple cubic Bravais lattice, and it is described as a simple cubic lattice with a basis consisting of a cesium ion at the origin **0** and a chlorine ion at the cube center $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

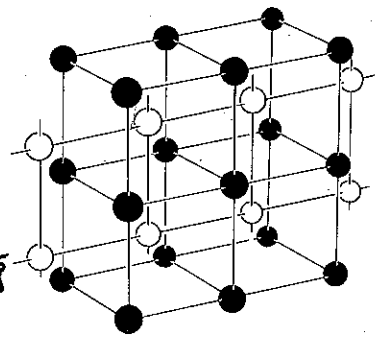


Figure 4.25
The cesium chloride structure. One type of ion is represented by black balls, the other type by white. The black and white balls form interpenetrating simple cubic lattices.

Table 4.6
SOME COMPOUNDS WITH THE CESIUM CHLORIDE STRUCTURE

CRYSTAL	a (Å)	CRYSTAL	a (Å)
CsCl	4.12	TlCl	3.83
CsBr	4.29	TlBr	3.97
CsI	4.57	TlI	4.20

The Zincblende Structure

Zincblende has equal numbers of zinc and sulfur ions distributed on a diamond lattice so that each has four of the opposite kind as nearest neighbors (Figure 4.18). This structure[19] is an example of a lattice with a basis, which must be so described both because of the geometrical position of the ions and because two types of ions occur.

Table 4.7
SOME COMPOUNDS WITH THE ZINCBLENDE STRUCTURE

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

[18] For examples see Table 4.6.
[19] For examples see Table 4.7.

DIAMOND & ZINCBLENDE

DIAMOND

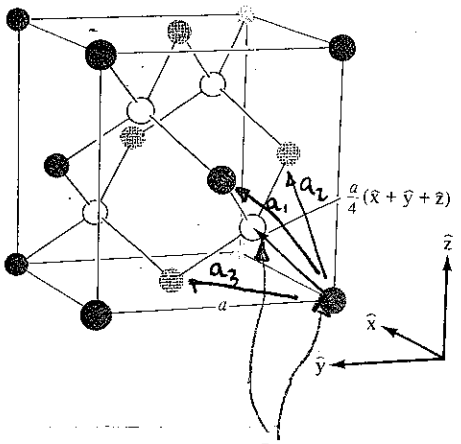


Table 4.3
ELEMENTS WITH THE DIAMOND CRYSTAL STRUCTURE

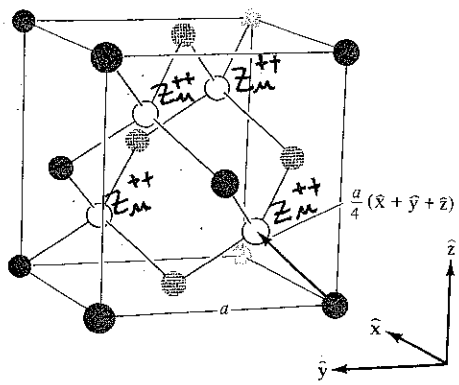
ELEMENT	CUBE SIDE a (Å)
C (diamond)	3.57 ← both
Si	5.43
Ge	5.66
α-Sn (grey)	6.49

FCC $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$ + BASIS (2)

BASIS

$(0,0,0), \frac{a}{4}(1,1,1)$

ZINCBLENDE



$Zn^{++}S^{--}$

IONIC ↔ ZnS

BASIS

$(0,0,0)$ SULFUR

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

which GaAs (SEMICONDUCTOR)

CdTe (QUANTUM DOTS)

~~ZnO~~ ZrO_2

CaF_2

$MX_2 \Rightarrow$ M = FCC

X are 8 interstitial sites cubic

ASSIGNMENT

~~FLUORITE~~ (96)

CRYSTOBALITE (92-93)

METHANE SOLID (94)

POLYETHYLENE (95-95)

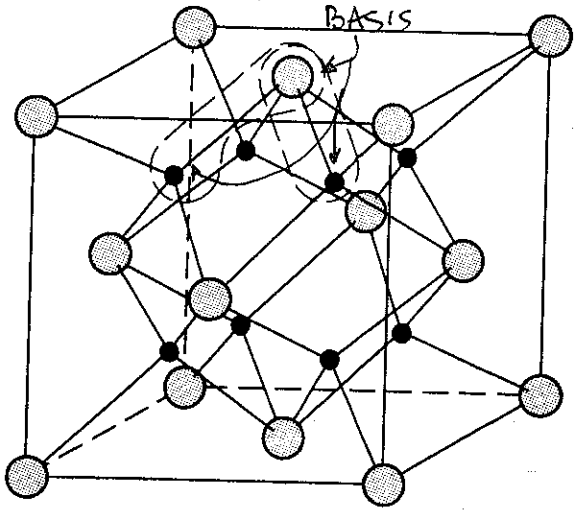
LIQUID CRYSTALS

(long molecules that can orient on some external field (ELECTRIC)

C24

FLUORITE - ANTIFLUORITE

ANION
● X ions
◯ M ions
METAL

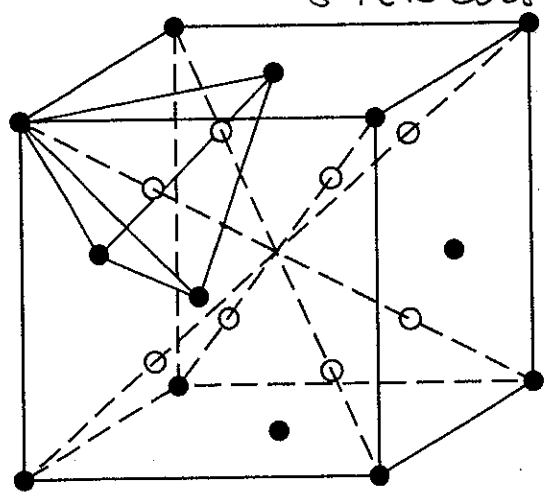


FLUORITE
= FCC + INTERSTITIAL
= FCC + BASIS (2)

twice as many interstitials

CaF_2, ~~ZrO_2~~, MX_2
4 — ↑ 2 ION
Metal

Tetrahedral site
INTERSTITIAC
8 PER CUBE



METAL
↙
M_2X
↖ ION

ANTIFLUORITE
Same as FLUORITE
BUT METAL INVERTED

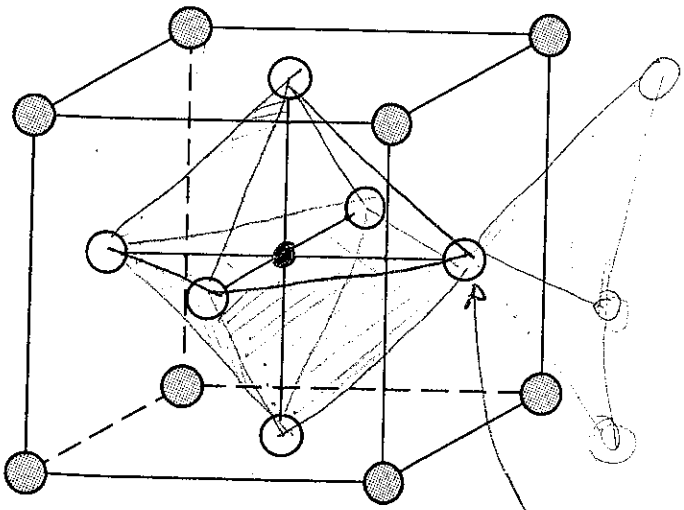
Li_2O,

PEROVSKITE STRUCTURE

USUALLY ABO_3

A, B metals

O oxygen



CUBIC

- Ti^{4+}
- Ca^{2+}
- O^{2-}

Oxygen takes all electrons O^{2-}

one metal gives 4

the other gives 2

$CaTiO_3$

CALCIUM TITANATE

SHARE CORNERS

a total of 6 electrons must come from the metals

CUBIC CALCIUM (A) STRUCTURE

OXIGEN IN THE FACES (6) ⟹ OCTAHEDRA

METAL TITANIUM (B) IN THE CENTRE

$LiCoO_3$ in BATTERIES

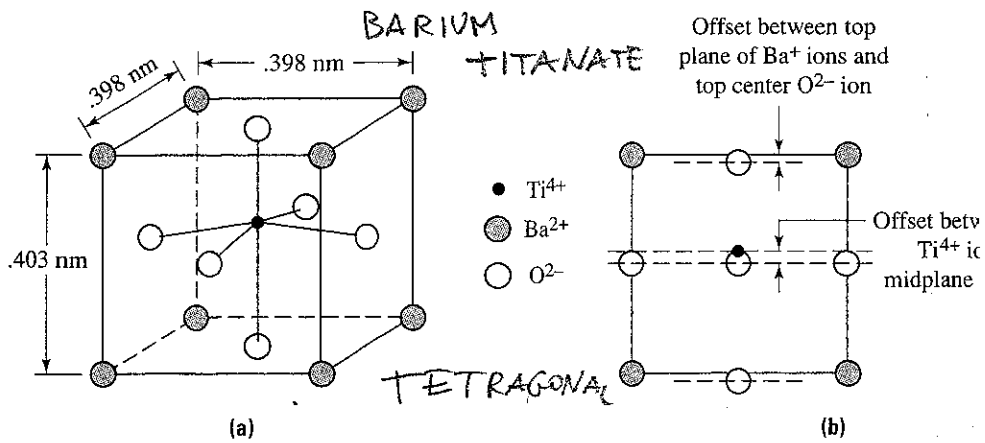
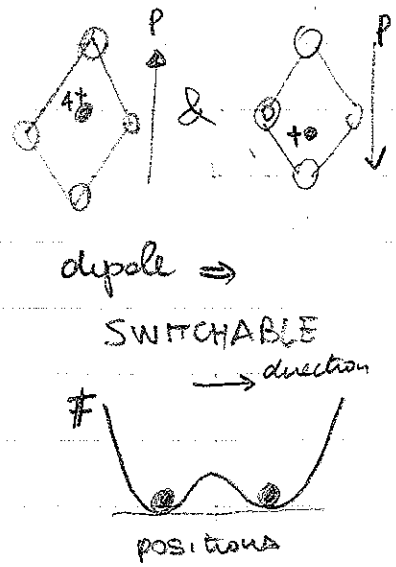


FIGURE 3.7–8 The tetragonal unit cell of $BaTiO_3$ shown **(a)** in 3-D, and **(b)** in 2-D.



C26

POLYCRISTALLINE

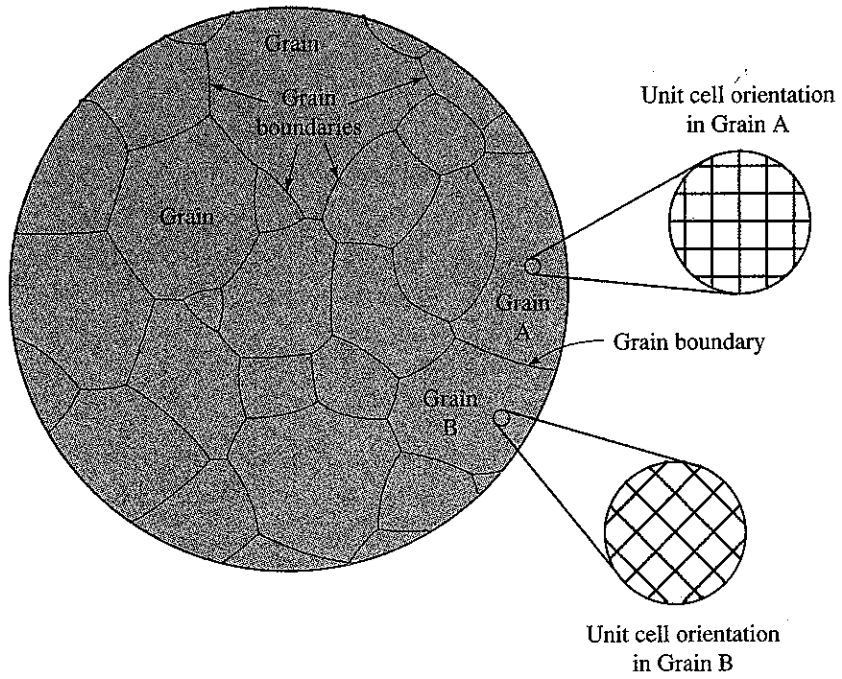


FIGURE 3.9–1
A schematic illustration of a polycrystalline sample. The polycrystal is composed of many grains separated by thin regions of disorder known as grain boundaries. Note that the unit-cell alignment within grain A (shown in the high-magnification insert) is different from that in grain B.

Many ceramic materials are also in the form of polycrystalline solids. With s inorganic solids, such as silica, it can be relatively easy to cool the material sufficie quickly that crystal formation does not occur. Hence, these materials may be ei crystalline or noncrystalline (amorphous), depending on thermal history. The structu noncrystalline and partially crystalline materials will be discussed in Chapter 6.

Polymers are unique in that because of the nature of long-chain molecules, they ra form structures that are entirely crystalline. Hence, polymers are either semicrysta or amorphous. Although there are no commercial single-crystal polymers, Spectra® f one of the strongest materials known, has a structure similar to that of a single cry Spectra consists of long polyethylene chains that are processed in such a way tha molecules are highly aligned. Crystallinity is very high, and defects, principally c ends, are randomly dispersed through the continuous crystal.

Few materials are used in a single-crystal form; however, those few are commerc significant. Single-crystal materials have no grain boundaries, so they offer unique chanical, optical, and electrical properties. Single-crystal quartz (SiO_2) and perovs are used as transducers in a variety of applications, such as in high quality receivers pickups (phonograph cartridges). Single-crystal germanium and silicon are used e sively in the microelectronics industry. Single-crystal nickel alloys are used in tu blades in high-performance jet aircraft. Sapphire (Al_2O_3) and diamond (C) single cry are precious stones.

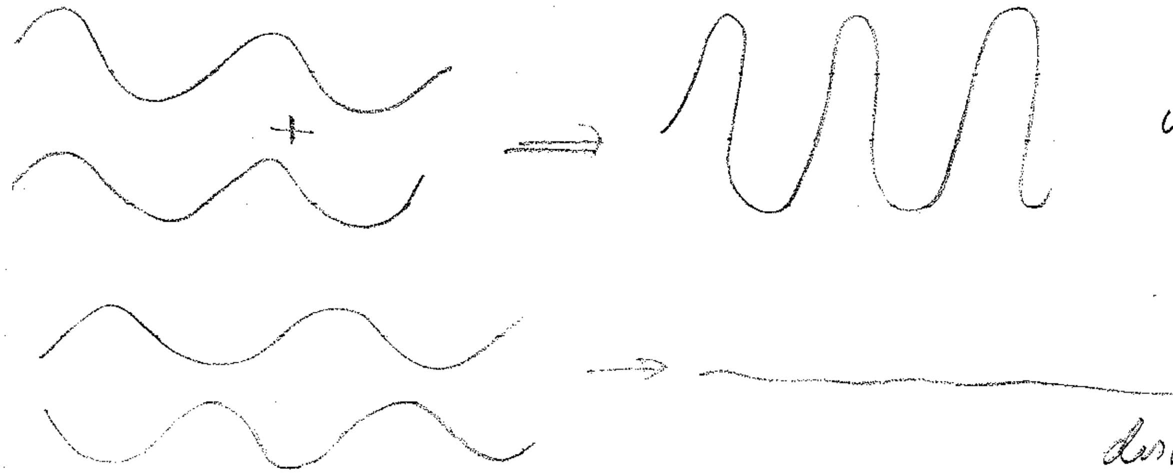
C27

3.10 ALLOTROPY AND POLYMORPHISM

Many materials can exhibit crystal structures that change from one unit cell to an

X-RAY DIFF (LIGHT)

in phase



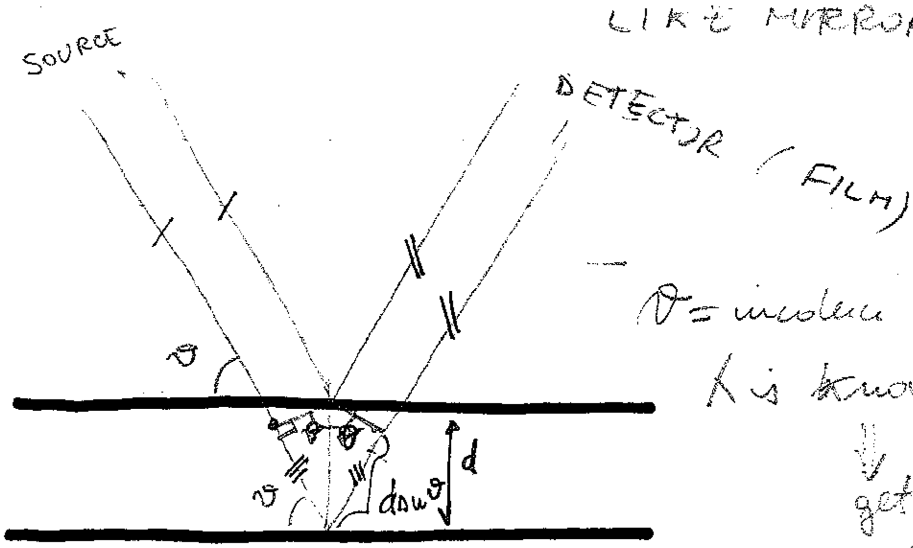
constructive interference

out of phase

destructive

phase or antiphase: depends on the distance traveled

ON A CRISTAL, PLANES REFLECT LIKE MIRRORS



θ = incidence angle

λ is known ⇒ get d

(path + path) = 2 d sin θ = extra distance

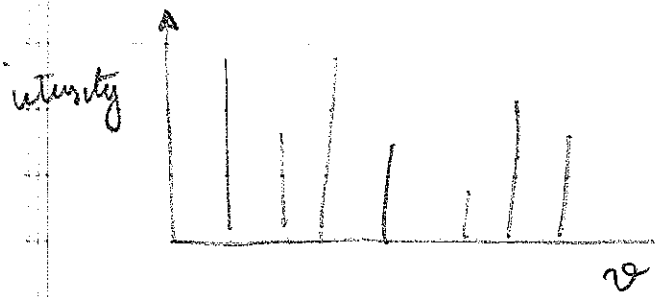
if this distance = nλ ⇒ positive interference

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

C28

But which plane am I toting?
DUNNO!

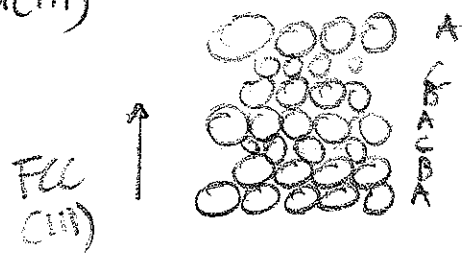
⇒ make powder ⇒ grind crystal and X-RAY POWDER

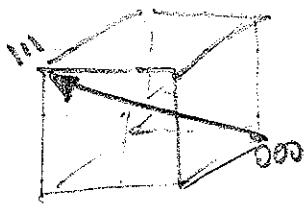


one for every plane

FCC

For instance $d(111)$

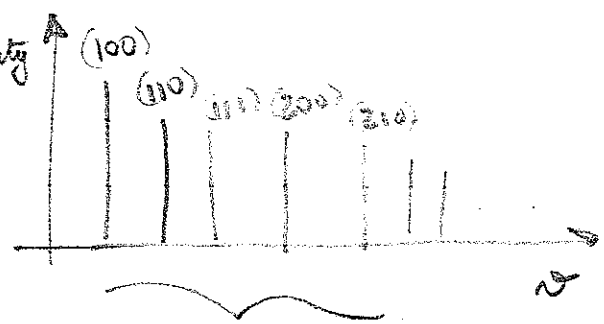




$a\sqrt{3}$

$$d(111) = \frac{a\sqrt{3}}{3}$$

for FCC $d(hkl) = \dfrac{a_0}{(h^2+k^2+l^2)^{1/2}}$ ⇒ formula of d_0 ⇒ formula of θ with position interplanar



line for every plane.

IF SOMETHING IS MISSING?

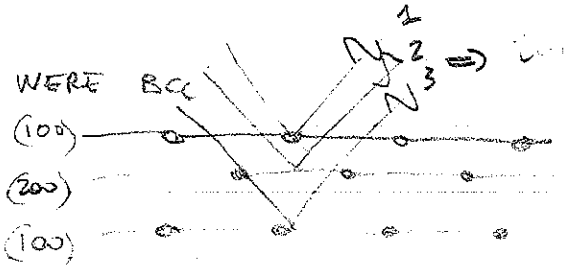
WHAT ABOUT MISSING LINES

EXAMPLE

TAKE CUBIC @ $\theta, \lambda \propto$ YOU HAVE LINE for d(100)

⇒ second ray has extra path $= n\lambda$

IF IT WERE BCC



3 ray has extra $n\lambda$
but 2 ray has $n\lambda/2$

⇒ DESTRUCTIVE DIFFRACTION

same for FCC (100)

⇒ RULES BCC: $(h+k+\ell)$ even ⇒ LINE (h,k,ℓ)
FCC: h,k,ℓ all even OR all odd (h,k,ℓ)

ALL X-RAY TECHNOLOGY IS AN EVOLUTION OF THESE IDEAS

⇒ EXTREMELY POWERFUL

Rvalue = $\frac{a^3}{2 \;\; 4}$ (2 ↑ BCC, 4 ↑ FCC)

STEFANO CURTAROLO MIT

MILTON COLE PHYSICS DEPT. 104 Davey Lab

LEGEND

MAGNESIUM		24.305
1.74	Mg	12
	[Ne] $3s^2$	
3.21	HEX	1.624
922		318

- Name: MAGNESIUM
- Symbol: Mg
- Mass Number: 24.305
- Density (gm cm^{-3}) (Common Crystal phase): 1.74
- Atomic Number: 12
- Atomic Configuration: [Ne] $3s^2$
- Lattice Constant, a (Å): 3.21
- Crystal Type (Common Crystal Phase): HEX
- c/a Ratio or Angle α in RHL (see Ch. 7) and b/a Ratio in ORC: 1.624
- Melting Temperature (K): 922
- Mean Debye Temperature (^{LT} signifies a low temperature determination): 318

FCC – Face-Centered Cubic
BCC – Body-Centered Cubic
SC – Simple Cubic
CUB – Cubic
TET – Tetragonal
ORC – Orthorhombic
HEX – Hexagonal
DIA – Diamond
RHL – Rhombohedral
MCL – Monoclinic

Periodic Table

Period	Group	Name	Mass Number	Density	Symbol	Atomic Number	Atomic Configuration	Lattice Constant	Crystal Type	c/a, angle or b/a	Melting Temperature	Debye Temperature
1	1A	HYDROGEN	1.0079	0.089	H	1	$1s^1$	3.75	HEX	1.731	14.0	110
1	Noble Elements	HELIUM	4.0026	0.179	He	2	$1s^2$	3.57	HEX	1.633	~1.0 (26 Atm)	26^{LT}
2	1A	LITHIUM	6.941	0.53	Li	3	$1s^22s^1$	3.49	BCC		453	400
2	2A	BERYLLIUM	9.0122	1.85	Be	4	$1s^22s^2$	2.29	HEX	1.567	1550	1000
2	3A	BORON	10.81	2.34	B	5	$1s^22s^22p^1$	8.73	TET	0.576	2600	1250
2	4A	CARBON	12.01	2.26	C	6	$1s^22s^22p^2$	3.57	DIA		(4300)	1860
2	5A	NITROGEN	14.007	1.03	N	7	$1s^22s^22p^3$	4.039	HEX	1.651	63.3	(β) 79^{LT}
2	6A	OXYGEN	15.999	1.43	O	8	$1s^22s^22p^4$	6.83	CUB		54.7	(γ) 46^{LT}
2	7A	FLUORINE	18.998	1.97 (α)	F	9	$1s^22s^22p^5$		MCL		53.5	
2	Noble Elements	NEON	20.18	1.56	Ne	10	$1s^22s^22p^6$	4.43	FCC		24.5	63
3	1A	SODIUM	22.9898	0.97	Na	11	[Ne] $3s^1$	4.23	BCC		371.0	150
3	2A	MAGNESIUM	24.305	1.74	Mg	12	[Ne] $3s^2$	3.21	HEX	1.624	922	318
3	3A	ALUMINUM	26.982	2.70	Al	13	[Ne] $3s^23p^1$	4.05	FCC		933	394
3	4A	SILICON	28.086	2.33	Si	14	[Ne] $3s^23p^2$	5.43	DIA		1683	625
3	5A	PHOSPHORUS	30.974	1.82 (white)	P	15	[Ne] $3s^23p^3$	7.17	CUB		317.3	
3	6A	SULFUR	32.064	2.07	S	16	[Ne] $3s^23p^4$	10.47	ORC	2.339 / 1.229	386	
3	7A	CHLORINE	35.453	2.09	Cl	17	[Ne] $3s^23p^5$	6.24	ORC	1.324 / 0.718	172.2	
3	Noble Elements	ARGON	39.948	1.78	Ar	18	[Ne] $3s^23p^6$	5.26	FCC		83.9	85
4	1A	POSTASSIUM	39.09	0.86	K	19	[Ar] $4s^1$	5.23	BCC		337	100
4	2A	CALCIUM	40.08	1.54	Ca	20	[Ar] $4s^2$	5.58	FCC		1111	230
4	3B	SCANDIUM	44.956	2.99	Sc	21	[Ar] $3d^14s^2$	3.31	HEX	1.594	1812	359^{LT}
4	4B	TITANIUM	47.90	4.51	Ti	22	[Ar] $3d^24s^2$	2.95	HEX	1.588	1933	380
4	5B	VANADIUM	50.942	6.1	V	23	[Ar] $3d^34s^2$	3.02	BCC		2163	390
4	6B	CHROMIUM	52.00	7.19	Cr	24	[Ar] $3d^54s^1$	2.88	BCC		2130	460
4	7B	MANGANESE	54.938	7.43	Mn	25	[Ar] $3d^54s^2$	8.89	CUB		1518	400
4	8	IRON	55.85	7.86	Fe	26	[Ar] $3d^64s^2$	2.87	BCC		1808	420
4	8	COBALT	58.93	8.9	Co	27	[Ar] $3d^74s^2$	2.51	HEX	1.622	1768	385
4	8	NICKEL	58.71	8.9	Ni	28	[Ar] $3d^84s^2$	3.52	FCC		1726	375
4	1B	COPPER	63.55	8.96	Cu	29	[Ar] $3d^{10}4s^1$	3.61	FCC		1356	315
4	2B	ZINC	65.38	7.14	Zn	30	[Ar] $3d^{10}4s^2$	2.66	HEX	1.856	693	234
4	3A	GALLIUM	69.72	5.91	Ga	31	[Ar] $3d^{10}4s^23p^1$	4.51	ORC	1.695 / 1.001	303	240
4	4A	GERMANIUM	72.59	5.32	Ge	32	[Ar] $3d^{10}4s^24p^2$	5.66	DIA		1211	360
4	5A	ARSENIC	74.922	5.72	As	33	[Ar] $3d^{10}4s^24p^3$	4.13	RHL	54°10′	1090	285
4	6A	SELENIUM	78.96	4.79	Se	34	[Ar] $3d^{10}4s^24p^4$	4.36	HEX	1.136	490	150^{LT}
4	7A	BROMINE	79.91	4.10	Br	35	[Ar] $3d^{10}4s^24p^5$	6.67	ORC	1.307 / 0.672	266	
4	Noble Elements	KRYPTON	83.80	3.07	Kr	36	[Ar] $3d^{10}4s^24p^6$	5.72	FCC		116.5	73^{LT}
5	1A	RUBIDIUM	85.47	1.53	Rb	37	[Kr] $5s^1$	5.59	BCC		312	56^{LT}
5	2A	STRONTIUM	87.62	2.60	Sr	38	[Kr] $5s^2$	6.08	FCC		1043	147^{LT}
5	3B	YTTRIUM	88.91	4.48	Y	39	[Kr] $4d^15s^2$	3.65	HEX	1.571	1796	258^{LT}
5	4B	ZIRCONIUM	91.22	6.49	Zr	40	[Kr] $4d^25s^2$	3.23	HEX	1.593	2125	250
5	5B	NIOBIUM	92.91	8.4	Nb	41	[Kr] $4d^45s^1$	3.30	BCC		2741	275
5	6B	MOLYBDENUM	95.94	10.2	Mo	42	[Kr] $4d^55s^1$	3.15	BCC		2890	380
5	7B	TECHNETIUM	98.91	11.5	Tc	43	[Kr] $4d^55s^2$	2.74	HEX	1.604	2445	
5	8	RUTHENIUM	101.07	12.2	Ru	44	[Kr] $4d^75s^1$	2.70	HEX	1.584	2583	382^{LT}
5	8	RHODIUM	102.90	12.4	Rh	45	[Kr] $4d^85s^1$	3.80	FCC		2239	350^{LT}
5	8	PALLADIUM	106.40	12.0	Pd	46	[Kr] $4d^{10}5s^0$	3.89	FCC		1825	275
5	1B	SILVER	107.87	10.5	Ag	47	[Kr] $4d^{10}5s^1$	4.09	FCC		1234	215
5	2B	CADMIUM	112.40	8.65	Cd	48	[Kr] $4d^{10}5s^2$	2.98	HEX	1.886	594	120
5	3A	INDIUM	114.82	7.31	In	49	[Kr] $4d^{10}5s^25p^1$	4.59	TET	1.078	429.8	129
5	4A	TIN	118.69	7.30	Sn	50	[Kr] $4d^{10}5s^25p^2$	5.82	TET	0.546	505	170
5	5A	ANTIMONY	121.75	6.62	Sb	51	[Kr] $4d^{10}5s^25p^3$	4.51	RHL	57°6′	904	200
5	6A	TELLURIUM	127.60	6.24	Te	52	[Kr] $4d^{10}5s^25p^4$	4.45	HEX	1.330	723	139^{LT}
5	7A	IODINE	126.90	4.94	I	53	[Kr] $4d^{10}5s^25p^5$	7.27	ORC	1.347 / 0.659	387	
5	Noble Elements	XENON	131.30	3.77	Xe	54	[Kr] $4d^{10}5s^25p^6$	6.20	FCC		161.3	55^{LT}
6	1A	CESIUM	132.91	1.90	Cs	55	[Xe] $6s^1$	6.05	BCC		302	40^{LT}
6	2A	BARIUM	137.34	3.5	Ba	56	[Xe] $6s^2$	5.02	BCC		998	110^{LT}
6	3B	LANTHANUM	138.91	6.17	La	57	[Xe] $5d^16s^2$	3.75	HEX	1.619	1193	132
6	4B	HAFNIUM	178.49	13.1	Hf	72	[Xe] $4f^{14}5d^26s^2$	3.20	HEX	1.582	2495	
6	5B	TANTALUM	180.95	16.6	Ta	73	[Xe] $4f^{14}5d^36s^2$	3.31	BCC			225
6	6B	TUNGSTEN (WOLFRAM)	183.85	19.3	W	74	[Xe] $4f^{14}5d^46s^2$	3.16	BCC		3683	310
6	7B	RHENIUM	186.2	21.0	Re	75	[Xe] $4f^{14}5d^56s^2$	2.76	HEX	1.615	3453	416^{LT}
6	8	OSMIUM	190.20	22.6	Os	76	[Xe] $4f^{14}5d^66s^2$	2.74	HEX	1.579	3318	400^{LT}
6	8	IRIDIUM	192.22	22.5	Ir	77	[Xe] $4f^{14}5d^76s^2$	3.84	FCC		2683	430
6	8	PLATINUM	195.09	21.4	Pt	78	[Xe] $4f^{14}5d^{10}6s^0$	3.92	FCC		2045	230
6	1B	GOLD	196.97	19.3	Au	79	[Xe] $4f^{14}5d^{10}6s^1$	4.08	FCC		1337	170
6	2B	MERCURY	200.59	13.6	Hg	80	[Xe] $4f^{14}5d^{10}6s^2$	2.99	RHL	70°45′	234.3	100
6	3A	THALLIUM	204.37	11.85	Tl	81	[Xe] $4f^{14}5d^{10}6s^26p^1$	3.46	HEX	1.599	577	96
6	4A	LEAD	207.19	11.4	Pb	82	[Xe] $4f^{14}5d^{10}6s^26p^2$	4.95	FCC		601	88
6	5A	BISMUTH	208.98	9.8	Bi	83	[Xe] $4f^{14}5d^{10}6s^26p^3$	4.75	RHL	57°14′	544.5	120
6	6A	POLONIUM	210	9.4	Po	84	[Xe] $4f^{14}5d^{10}6s^26p^4$	3.35	SC		527	
6	7A	ASTATINE	210		At	85	[Xe] $4f^{14}5d^{10}6s^26p^5$				(575)	
6	Noble Elements	RADON	222	(4.4)	Rn	86	[Xe] $4f^{14}5d^{10}6s^26p^6$		(FCC)		(202)	
7	1A	FRANCIUM	223		Fr	87	[Rn] $7s^1$		(BCC)		(300)	
7	2A	RADIUM	226	(5.0)	Ra	88	[Rn] $7s^2$				973	
7	3B	ACTINIUM	227	10.1	Ac	89	[Rn] $6d^17s^2$	5.31	FCC		1323	

RARE EARTHS

LANTHANIDES 6

Name	Mass Number	Density	Symbol	Atomic Number	Atomic Configuration	Lattice Constant	Crystal Type	c/a or angle	Melting Temperature	Debye Temperature
CERIUM	140.12	6.77	Ce	58	[Xe] $4f^25d^06s^2$	5.16	FCC		1071	139^{LT}
PRASEODYMIUM	140.91	6.77	Pr	59	[Xe] $4f^35d^06s^2$	3.67	HEX	1.614	1204	152^{LT}
NEODYMIUM	144.24	7.00	Nd	60	[Xe] $4f^45d^06s^2$	3.66	HEX	1.614	1283	157^{LT}
PROMETHIUM	145		Pm	61	[Xe] $4f^55d^06s^2$				(1350)	
SAMARIUM	150.35	7.54	Sm	62	[Xe] $4f^65d^06s^2$	9.00	RHL	23°13′	1345	166
EUROPIUM	151.96	7.90	Eu	63	[Xe] $4f^75d^06s^2$	4.61	BCC		1095	107^{LT}
GADOLINIUM	157.25	8.23	Gd	64	[Xe] $4f^75d^16s^2$	3.64	HEX	1.588	1585	176^{LT}
TERBIUM	158.92	8.54	Tb	65	[Xe] $4f^95d^06s^2$	3.60	HEX	1.581	1633	188^{LT}
DYSPROSIUM	162.50	8.78	Dy	66	[Xe] $4f^{10}5d^06s^2$	3.59	HEX	1.573	1680	186^{LT}
HOLMIUM	164.93	9.05	Ho	67	[Xe] $4f^{11}5d^06s^2$	3.58	HEX	1.570	1743	191^{LT}
ERBIUM	167.26	9.37	Er	68	[Xe] $4f^{12}5d^06s^2$	3.56	HEX	1.570	1795	195^{LT}
THULIUM	168.93	9.31	Tm	69	[Xe] $4f^{13}5d^06s^2$	3.54	HEX	1.570	1818	200^{LT}
YTTERBIUM	173.04	6.97	Yb	70	[Xe] $4f^{14}5d^06s^2$	5.49	FCC		1097	118^{LT}
LUTETIUM	174.97	9.84	Lu	71	[Xe] $4f^{14}5d^16s^2$	3.51	HEX	1.585	1929	207^{LT}

ACTINIDES 7

Name	Mass Number	Density	Symbol	Atomic Number	Atomic Configuration	Lattice Constant	Crystal Type	c/a or b/a	Melting Temperature	Debye Temperature
THORIUM	232.04	11.7	Th	90	[Rn] $6d^27s^2$	5.08	FCC		2020	100
PROTACTINIUM	231	15.4	Pa	91	[Rn] $5f^26d^17s^2$	3.92	TET	0.825	1470	
URANIUM	238.03	19.07	U	92	[Rn] $5f^36d^17s^2$	2.85	ORC	2.056 / 1.736	1406	210^{LT}
NEPTUNIUM	237.05	20.3	Np	93	[Rn] $5f^56d^07s^2$	4.72	ORC	1.411 / 1.035	913	188^{LT}
PLUTONIUM	244	19.8	Pu	94	[Rn] $5f^66d^07s^2$		MCL		914	150^{LT}
AMERICIUM	243	11.8	Am	95	[Rn] $5f^76d^07s^2$				1267	
CURIUM	247		Cm	96	[Rn] $5f^76d^17s^2$				1600	
BERKELIUM	247		Bk	97	[Rn] $5f^76d^27s^2$					
CALIFORNIUM	251		Cf	98	[Rn] $5f^96d^17s^2$					
EINSTEINIUM	254		Es	99						
FERMIUM	257		Fm	100						
MENDELEVIUM	256		Md	101						
NOBELIUM	254		No	102						
LAWRENCIUM	257		Lw	103						