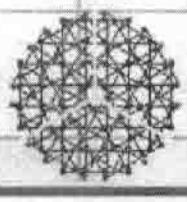
MSE170 U. Washington

Fundamentals of Materials Science



LAB II
CRYSTAL STRUCTURE

Study Questions:

1. What properties of a strongly bonded covalent solid like diamond can be attributed to its bond type? mechanical, electrical, optical, thermal

takeOut ~~2. How are these properties a result of chemical bonding?~~

2. Explain why covalent bonds are directional but ionic bonds are not. sharing (polarity) vs. transfer of e^-

3. Show the electron notation of Cu, Cu^{+1}, and Cu^{+2}. ① $[Ar]4s^1 3d^{10}$ ② $[Ar]4s^2 3d^8$ ③ $[Ar]4s^2 3d^7$

4. Explain why a simple ionic crystal like CsCl cannot crystallize into a BCC structure. two different atoms/ions

5. Graphite is very anisotropic; that is, its properties are dependent on crystallographic direction. Given a cross-section of graphite, try to explain why the electrical conductivity of graphite is 100 times greater in the horizontal direction than in the vertical. bonding – covalent within sheets, v.d.w. between sheets

see next page

6. Consider an FCC unit cell with the lattice parameter 'a'. Calculate the diameter of the atoms making up this unit cell.

7. For a cubic crystal system, how many ⟨110⟩ directions are contained in the (111) plane?

8. For a cubic crystal system, label the following: [100], (112), [123], and (123).

Lab:

I. Crystal Structure

A *lattice* is a regular array of points repeated through space. The *Bravais lattices* are the14 different lattices possible in 3-dimensional space. A crystal structure is a three dimensional arrangement of atoms or groups of atoms in space that can follow any of the 14 Bravais lattices. A primary unit cell is the smallest repeating unit of a crystal structure. Unit cells are parallelograms in two dimensions and parallelepipeds in three dimensions.

The size and shape of a unit cell is described, in three dimensions, by the lengths of the three edges (a, b, and c) and the angles between the edges (α, β, and γ). These quantities are referred to as the *lattice parameters* of the unit cell. For a cubic unit cell, a=b=c and $\alpha=\beta=\gamma=90°$. Note that although different materials may have the same unit cell and crystal structure, they will not have the same lattice parameters.

PART 2: CRYSTAL STRUCTURE

Study Questions:

1. What properties of a strongly bonded covalent solid like diamond can be attributed to its bond type?

   Mechanical, Thermal, Electrical, Optical ect

2. Explain why covalent bonds are directional but ionic bonds are not.

   Ionic – coulombic force between point charges. Sphereical electon distrobution around nucleus
   Covalent- Shared electrons between two specific atoms along a specific direction

3. Show the electron notation of Cu, Cu^{+1}, and Cu^{+2}.

   Cu $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
   Cu^{+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$
   Cu^{2+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$

4. Explain why a simple ionic crystal like CsCl cannot crystallize into a BCC structure.

   Two different types of atoms. (Could crystallize into Rock salt structure)

5. Graphite is very anisotropic; that is, its properties are dependent on crystallographic direction. Given a cross-section of graphite, try to explain why the electrical conductivity of graphite is 100 times greater in the horizontal direction than in the vertical.

   Covalent Bonding within Sheets, Van der Waals forces between sheets

6. Consider an FCC unit cell with the lattice parameter 'a'. Calculate the diameter of the atoms making up this unit cell.

   $d = a\sqrt{2}/2$

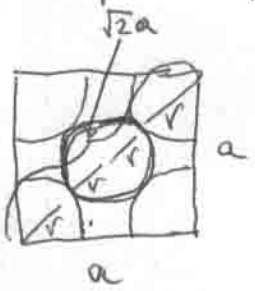
7. For a cubic crystal system, how many <110> directions are contained in the (111) plane?

6 directions in the <110> family of directions are in the (111) plane. 110, 101, 011, 110, 101, 011

8. For a cubic crystal system, label the following: [100], (112), [123], and (123).

Questions:

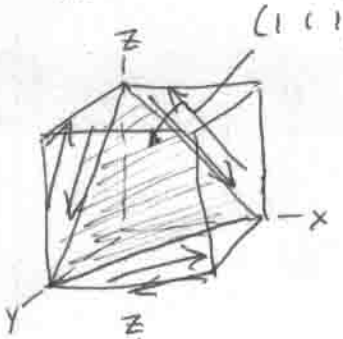
close-packed plane for FCC is {100}, close-packed direction <100>



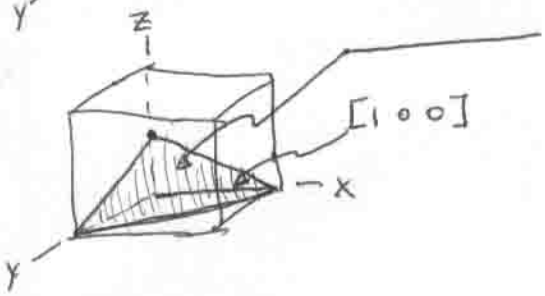
$4r = 2d = \sqrt{2}a$

$$\boxed{d = \frac{\sqrt{2}}{2}a}$$

(8) (1 1 1) ? <1 1 0> = 6 both ways count



(9)

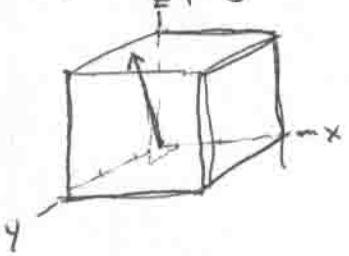


(1 1 2)

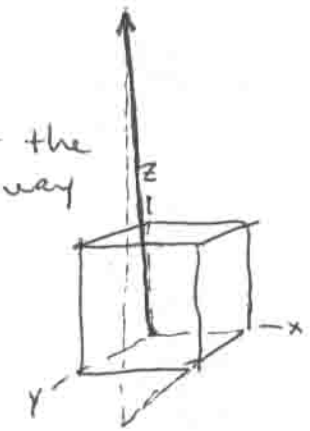
1 1 $\frac{1}{2}$ reciprocal to get intercepts

[1 2 3]

$\frac{1}{6}$ $\frac{1}{3}$ $\frac{1}{2}$ LCM to get projection

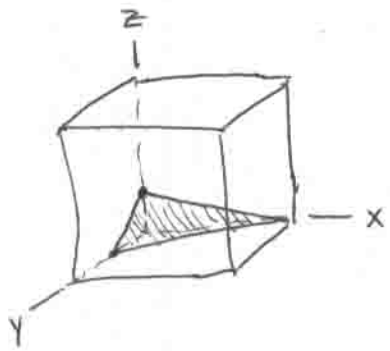


OR do it the long way

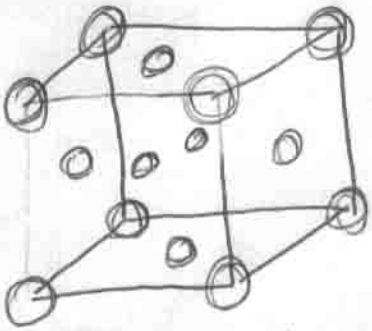


(1 2 3)

1 $\frac{1}{2}$ $\frac{1}{3}$ reciprocals to get intercepts

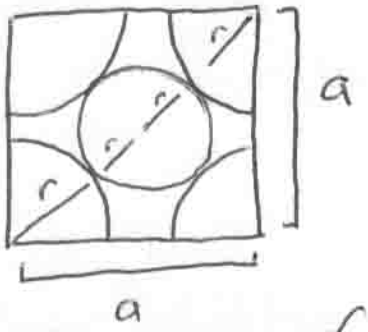


6.



FCC unit cell

one face off FCC unit cell



$4r = 2d$ ← diameter

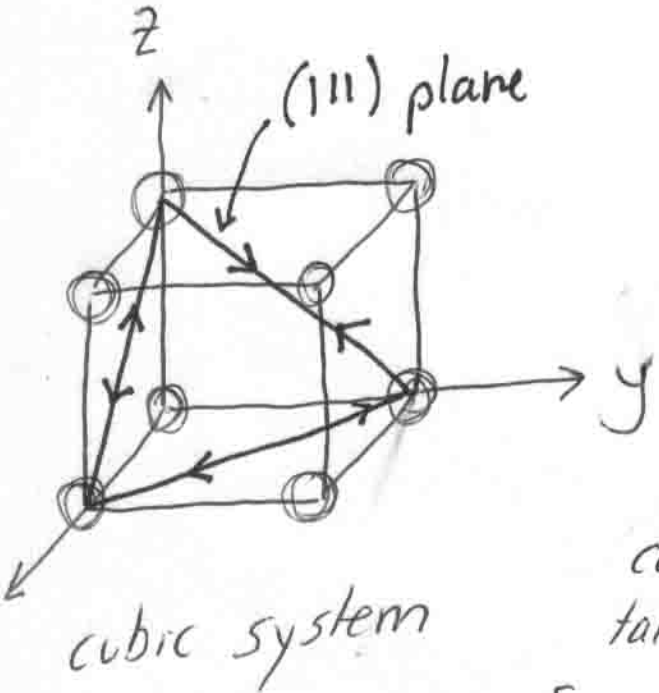
$(2d)^2 = a^2 + a^2$ from triangle

$4d^2 = 2a^2$

$d^2 = \frac{2a^2}{4}$

$d = \frac{a\sqrt{2}}{2}$

7.



cubic system

$\langle 110 \rangle$ family of directions

same atomic spacing along each direction.

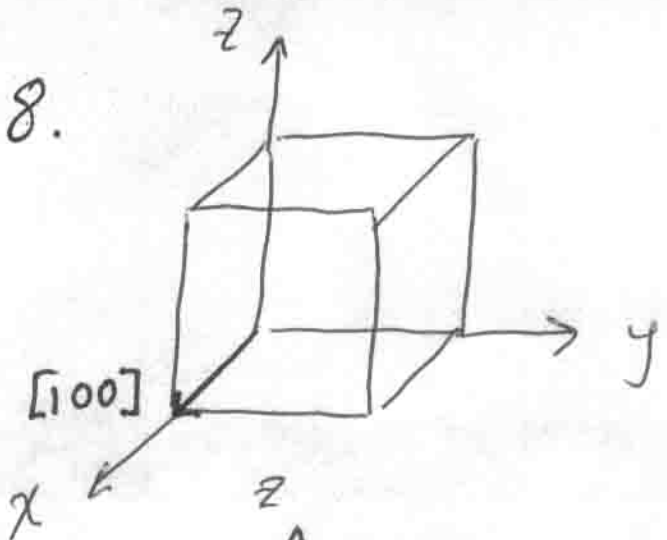
(In cubic system)

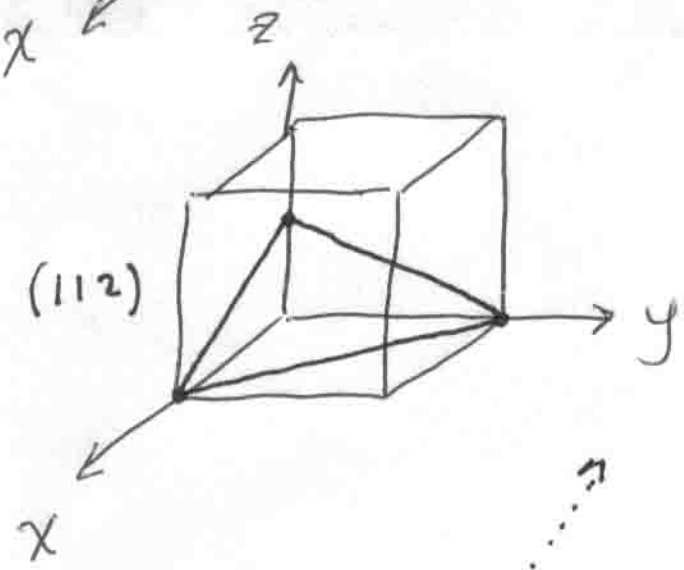
can rearrange indices and take negatives of indices

$[110]$ $[101]$ ~~$[011]$~~

negatives $[\bar{1}\bar{1}0]$ $[\bar{1}0\bar{1}]$ $[0\bar{1}\bar{1}]$

8.

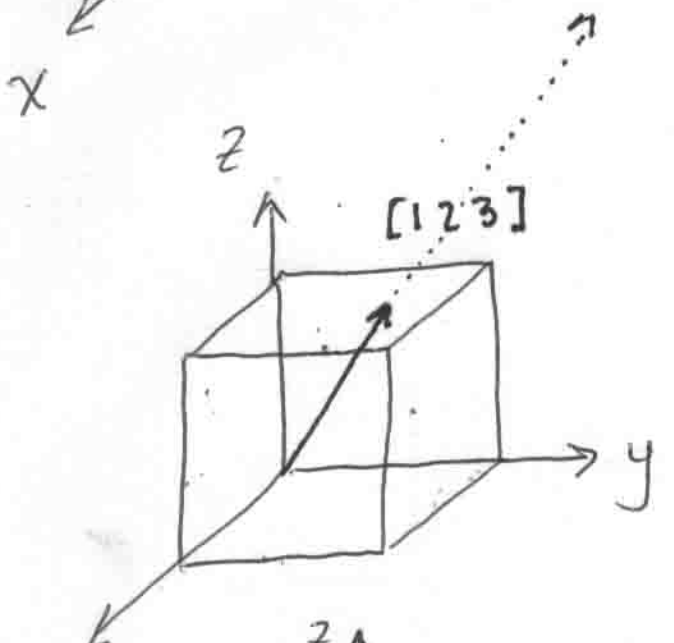




(1 1 2) plane → take reciprocals

(1 1 $\frac{1}{2}$) reciprocals

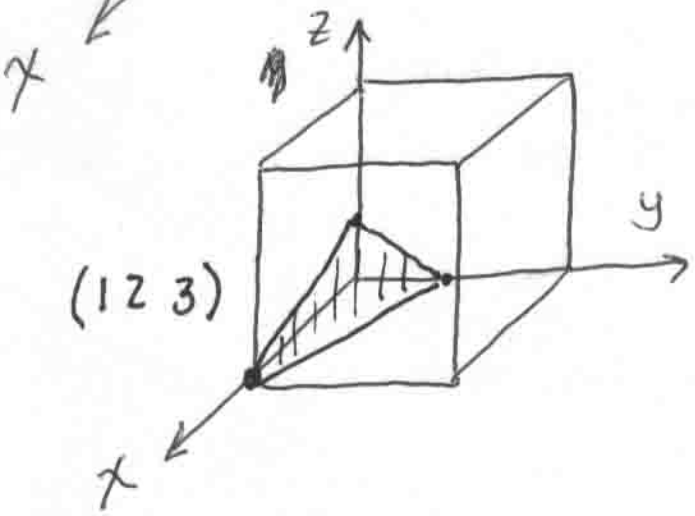
(1 1 $\frac{1}{2}$) ← intercepts



[1 2 3] direction →

~~1 2 3~~ divide by lowest common multiple (3)

$\frac{1}{3}$ $\frac{2}{3}$ $\frac{3}{3}$ to get direction in unit cell



(1 2 3) plane →

~~1~~ $\frac{1}{2}$ $\frac{1}{3}$ reciprocals

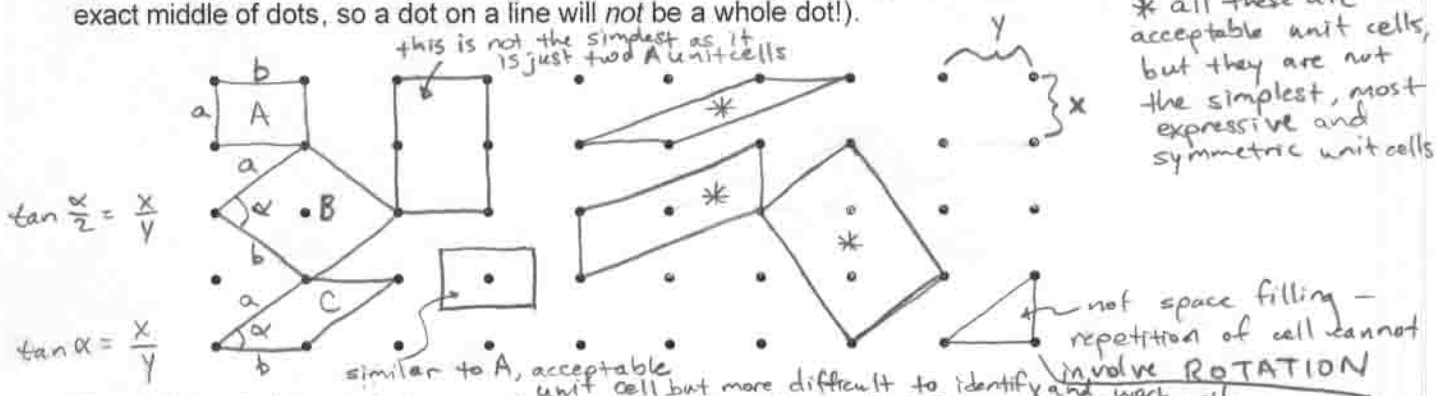
$\frac{1}{2}$ $\frac{1}{3}$ ← intercepts

I.1 What would explain the difference in lattice parameters between materials with the same crystal structure (e.g., BCC)?

Size of atoms

The selection of a unit cell is not unique; the corners of a unit cell may actually be any where within the space of the lattice, provided that repeated translations of this chosen cell will fill all of the space of the lattice. Conventional practice is to choose the smallest, simplest, most expressive and symmetric unit cell for the lattice.

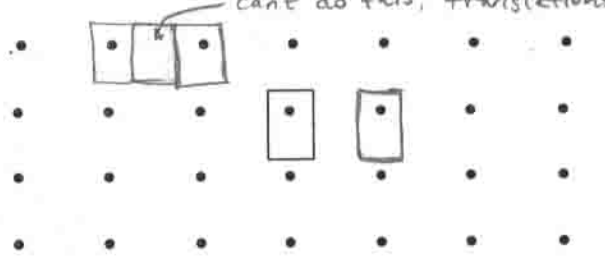
I.2 Here is a two-dimensional grid of dots. Draw 3 unique unit cells on this grid, with cell corners on dots, labeling the unit cells as A, B, and C, respectively. Next, determine each cell's lattice parameters a, b, and α (here, the smallest angle between any a and b). Finally, give the number of dots in each cell (assuming that any lines intersect the exact middle of dots, so a dot on a line will *not* be a whole dot!).



The horizontal distance between adjacent dots is 'x' and the vertical distance between adjacent dots is 'y'. Express 'a', 'b', and 'α' (if necessary) in terms of these.

unit cell	a	b	α	# dots in unit cell
A	x	y	90°	1
B	$\sqrt{x^2+y^2}$	$\sqrt{x^2+y^2}$	$2\tan^{-1}\frac{x}{y}$	2
C	$\sqrt{x^2+y^2}$	y	$\tan^{-1}\frac{x}{y}$	1

I.3 Other than not having its corners on dots, would the following cell be a valid unit cell? If not, why not?



No

Repetitions of the cell are not space filling

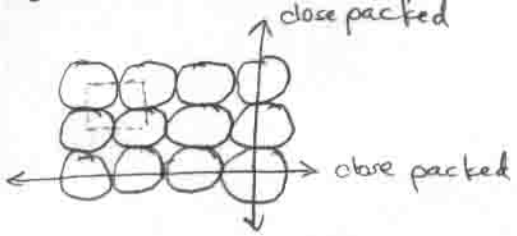
II. Two - Dimensional Packing

Use pennies to represent a two dimensional array of atoms. There are two basic configurations: square packing and close packing.

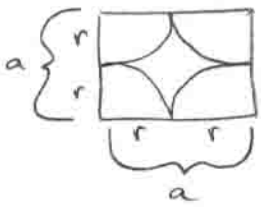
First, arrange the pennies into square packing and answer the following questions:

II.1 What is the coordination number (number of nearest neighbors or pennies touching) of one penny in this arrangement? 4

II.2 Draw the simplest unit cell (must be more than one penny!) for this packing configuration and indicate all close packed directions.



unit cell



II.3 What is its value for α? 90°

II.4 Give an expression for the unit cell lattice parameter 'a' in terms of penny radius 'r'.

a= 2r

II.5 Find the packing fraction (i.e., packing efficiency) for your unit cell: 78.5%
(defined as area of the atoms divided by the area of the unit cell)

$$P.F. = \frac{A_{atoms}}{A_{unit\,cell}} = \frac{\pi r^2}{(2r)(2r)} = 78.5\%$$

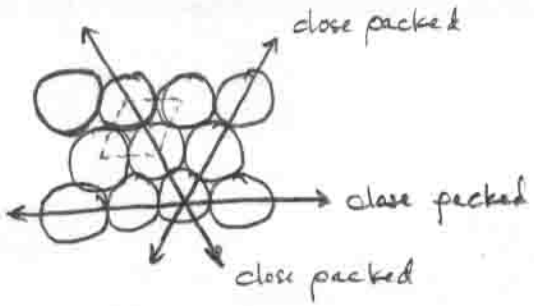
5 -1 for each done incorrectly

5

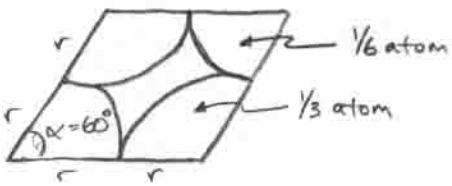
Now arrange the pennies into close packing and answer the following questions:

II.6 What is the coordination number (number of nearest neighbors or pennies touching) of one penny in this arrangement? 6

II.2 Draw the simplest unit cell (must be more than one penny!) for this packing configuration and indicate all close packed directions.

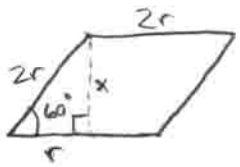


unit cell



II.8 What is its value for α? 60°

II.9 Give an expression for the unit cell lattice parameter 'a' in terms of penny radius 'r'.



$\frac{2r}{2} = \frac{x}{\sqrt{3}}$

$x = \sqrt{3}r$

a= 2r

II.10 Find the packing fraction (i.e., packing efficiency) for your unit cell: 90.7%
(defined as area of the atoms divided by the area of the unit cell)

$$P.F. = \frac{\pi r^2}{2r(\sqrt{3}r)} = 90.7\%$$

5 -1 for each done incorrectly

5

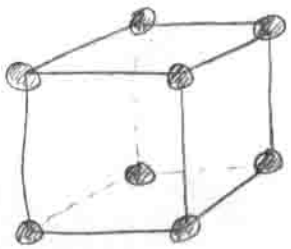
III. Three - Dimensional Packing

The four most basic crystal structures are:

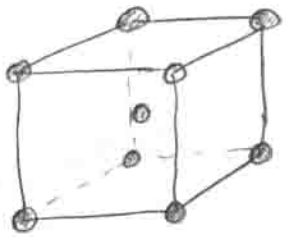
- Simple cubic (SC)
- Body centered cubic (BCC)
- Face centered cubic (FCC)
- Hexagonal close packed (HCP)

You should develop a complete understanding of the geometry and atomic arrangement of each of these structures. Make a sketch of each of these structures below.

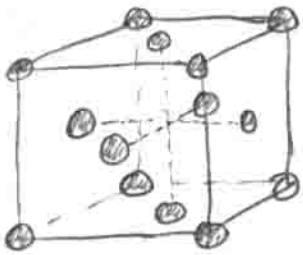
III.1 Simple Cubic



III.2 Body Centered Cubic

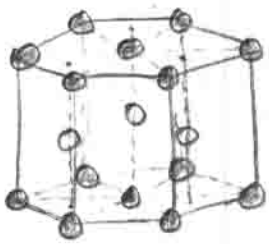


III.3 Face Centered Cubic



-1 for each incomplete

III.4 Hexagonal Close Packed



5

5

Now *construct* each of these four crystal structures using Styrofoam balls and toothpicks. You should strive to completely understand the atomic packing and geometry of each of these structures. Begin by creating the individual layers, and then stack each layer together to compose the structure. To test your understanding you should discuss the similarities and differences between the structures in your team. Be sure that you can completely visualize each structure.

III.5 For each structure determine the following:

homework
homework
review in class
homework

Structure	atoms/cell	coordination #	APF	a = f(r)
SC	1	6	0.52	$2r$
BCC	2	8	0.68	$4r/\sqrt{3}$
FCC	4	12	0.74	$2r\sqrt{2}$
HCP	6	12	0.74	$2r$

-1 each
16 total

FCC

$a^2 + a^2 = c^2$ ← the diagonal

$2a^2 = c^2$

$a\sqrt{2} = c$

$a\sqrt{2} = 4r$

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

2 pts

$$A.P.F = \frac{V_{\text{atoms in unit cell}}}{V_{\text{unit cell}}} = \frac{n\,V_{\text{one atom}}}{a^3} = \frac{(4)\left(\frac{4}{3}\pi r^3\right)}{(2r\sqrt{2})^3} = 0.74$$

(n = # of atoms per unit cell)

Which two structures show the greatest similarities? FCC and HCP

2 pts

20/

Consider the BCC and FCC structures you have built:

lower packing factor

2pts **III.6** Which crystal has the largest interstitial site? BCC FCC

2pts **III.7** Does the size of the interstitial sites in each crystal type correlate with APF? (i.e., does a higher APF mean smaller interstitial sites?) Yes No (# of interstitial sites) no correlation ~~↑APF ↓ interstitial size~~ ~~increase relation~~ ~~APF ↑ size structure~~

III.8 There are 2 different types of interstitial sites for BCC crystals. How many of each type are there? Indicate in a sketch where each is.

see diagrams next page

3pts sketch

III.9 There are 2 different types of interstitial sites for FCC crystals. How many of each type are there? Indicate in a sketch where each is.

3pts sketch see diagrams next page

have students find in book

III.10 If material properties (tensile strength, conductivity, etc) are a function of crystal structure, will the measured properties of some materials vary with crystal orientation? How can you explain this?

5pts ① Yes, will vary

5pts ② Specific close packed planes for a given structure Packing not the same in all directions → properties not same in all directions

Anisotropy p 46 in Callister

/20

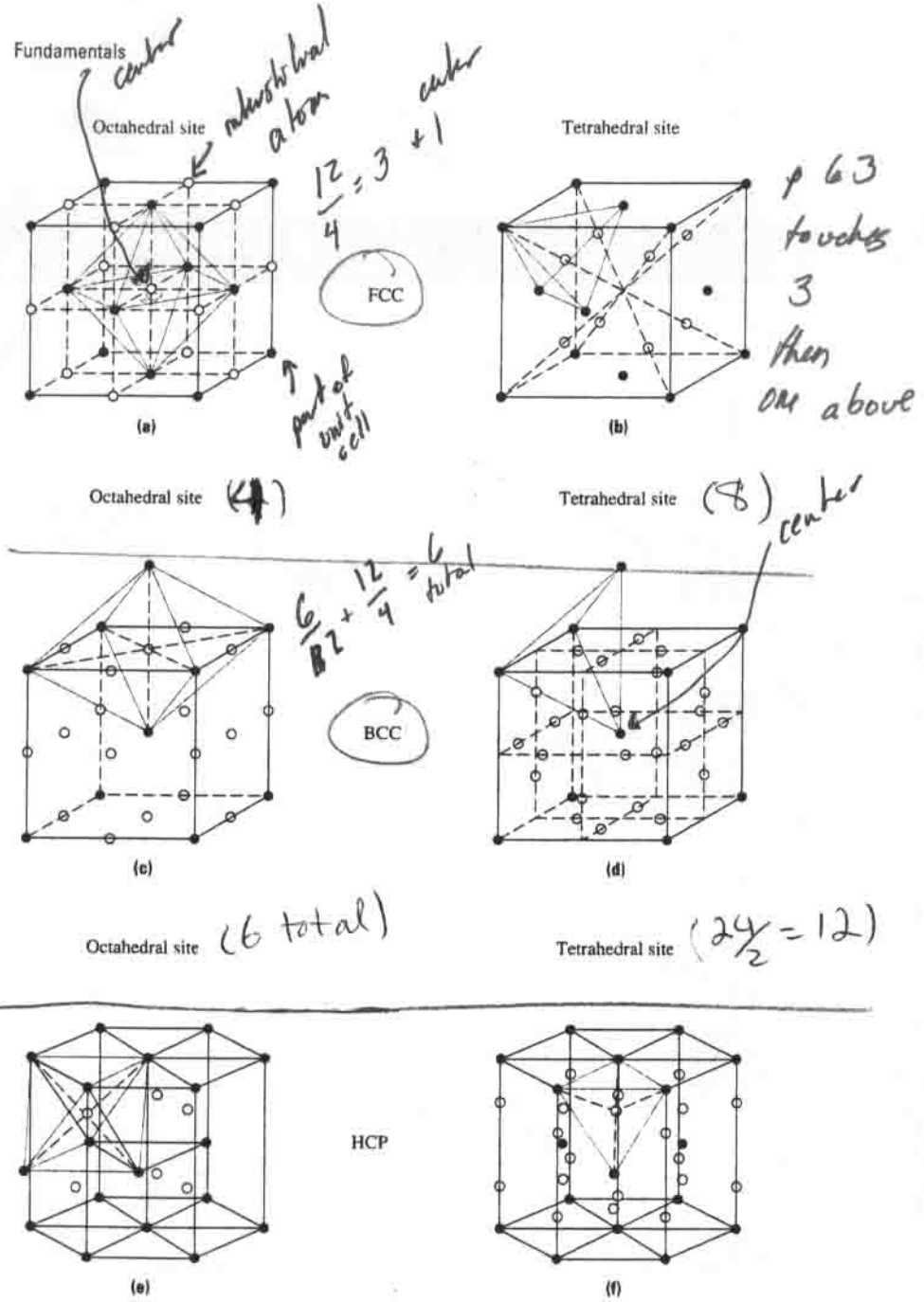


FIGURE 3.6–1
The locations of the interstitial sites in the common crystal structures: **(a)** octahedral sites in FCC, **(b)** tetrahedral sites in FCC, **(c)** octahedral sites in BCC, **(d)** tetrahedral sites in BCC, **(e)** octahedral sites in HCP, and **(f)** tetrahedral sites in HCP.

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

Homework

IV. Ionic Structure

Although we have been examining single element crystal structures, the same principles apply to ionic structures composed of two or more elements. In this case we find the bonding to be predominately ionic, rather than metallic or covalent, which has several implications.

In your textbook, there is a discussion of coordination numbers and geometries that are dependent on the cation-anion radius ratio in the ionic compound: r_c/r_a. Stable ceramic crystal structures form when anions that surround a cation are all in direct contact with the cation, and the coordination of that cation is related to the cation-anion radius ratio.

IV.1 Given an ionic radius for Na^+ ion = 0.95Å and for Cl^- = 1.81Å, what is the cation to anion radius ratio for NaCl?

★ 10pts.

$r_c/r_a = \frac{0.95}{1.81} = 0.52$ 10

IV.2 Referring to the range of radius ratios to coordination numbers (in Callister), what is the coordination number of the Na^+ ions in the NaCl structure?

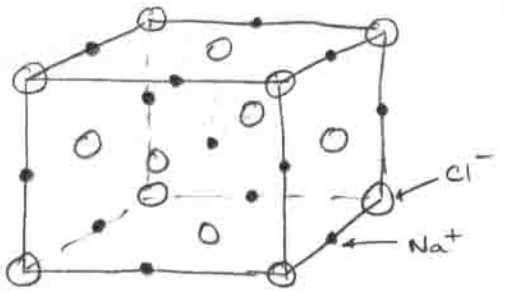
★ 10pts.

C# = 6 10

IV.3 Make a three dimensional sketch of the NaCl structure below, indicating which are the Na^+ and Cl^- ions. The ions should be roughly in scale relative to one another: that is, they should *not* be drawn having the same size.

10

★ 10pts.



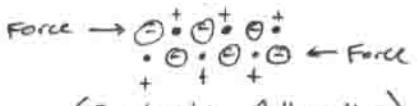
★2 pts. 2

IV.4 How many Na^+ ions are present within the cell? 4 How many Cl^- ions are present? 4 ★2 pts 2 Is there charge neutrality within the cell? YES ★ 1 pt. 1

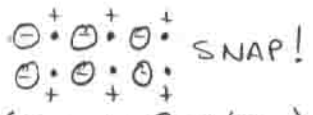
IV.5 How might you explain the brittle nature of ceramics? Consider that ceramic materials are composed of two or more ionic species, while metals are not. They both form similar crystal structures, why is one so much more brittle than the other?

★ 10 pts 10

Ionic Species Repel:



(Coulombic Attraction)



(Coulombic Repulsion)

* There will be some elastic deformation as bonds are strained but no plastic deformation

45