SEOUL NATIONAL UNIVERSITY
1 GWANAK-RO, GWANAK-GU, SEOUL, 08826, KOREA

1. (self-study question) Explain different types bonding of Hydrogen Bond, Ionic Bond, Covalent Bond, and Metalic Bond. (20 pt)

a) Ionic Bond

Ionic bonding involves a transfer of an electron, so one atom gains an electron while one atom loses an electron. One of the resulting ion carries a negative charge (anion), and the other ion carries a positive charge (cation). Because opposite charges attract, the atoms bond together to form a molecule. ✓

ex) NaCl : $Na\cdot + \cdot\ddot{Cl}: \rightarrow Na^+ + :\ddot{Cl}:^-$

b) Covalent Bond

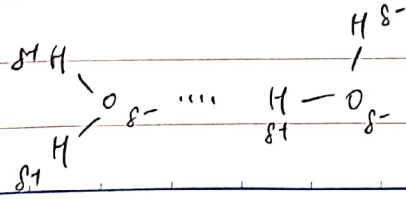
The most common bond in organic molecules, a covelent bond involves the sharing of electrons between two atoms. The pair of shared electrons forms a new orbit that extends around the nuclei of both atoms, producing a molecule. There are two secondary types of covalent bonds — polar bonds & hydrogen bonds ✓

ex) H_2 : $H\cdot + \cdot H \rightarrow H:H$ (H-H)

HCl : $H\cdot + \cdot\ddot{Cl}: \rightarrow H:\ddot{Cl}:$ (H-Cl)

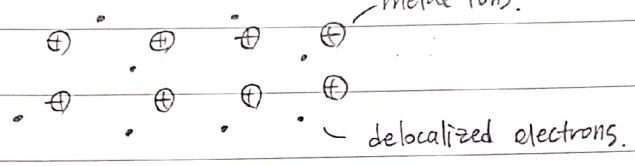
c) Hydrogen Bond

Because they're polarized, two adjacent H_2O molecules can form a linkage known as hydrogen bond, where the (electronegative) hydrogen atom of one H_2O molecule is electrostatically attracted to the (electropositive) oxygen atom of an adjacent water molecule. Consequently, molecules of water join together transiently in a hydrogen-bonded lattice. Hydrogen bonds have only about 1/20 strength of a covalent bond, yet even this force is sufficient to affect the structure of water, producing many of its properties, such as high surface tension, specific heat & heat of vaporization. ✓



d) Metallic Bond.

Metallic bonding rises from the electrostatic attractive force between conduction electrons (in the form of an electron cloud of delocalized electrons) and positively charged metal ions. It may be described as the sharing of free electrons among a structure of positively charged ions (cations). Metallic bonding accounts for many physical properties of metals, such as strength, ductility, thermal and electrical resistivity and conductivity ... Metallic bonding is not the only type of chemical bonding a metal can exist, even as a pure substance.



2. For simple cubic structure with single type of atom (C, carbon) and lattice parameter $a = 3.5\,\text{Å}$, calculate below properties : (10 pt)

a) packing density (volumetric portion of atoms in a unit cell volume)

b) Number of atoms of 1st nearest neighbors.

c) Distance of 1st nearest neighbors

solution)

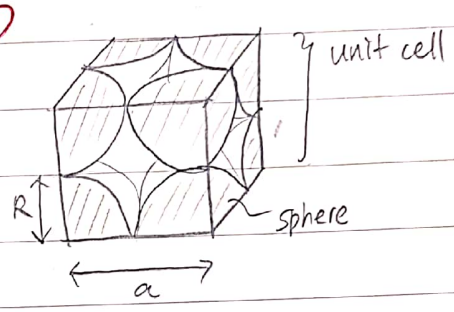
a) packing density of SC

$R \neq \frac{a}{2}$

-3

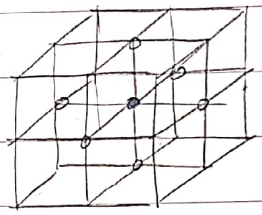
- packing density $= \dfrac{n \times V_{sphere}}{V_{unit\,cell}}$, $n = \frac{1}{8} \times 8 = 1$
- $V_{unit\,cell} = a^3$, $a = 2R$ $\therefore V_{unit\,cell} = 8R^3$
- $V_{sphere} = \frac{4}{3}\pi R^3$,

$\therefore$ packing density $= \dfrac{\frac{4}{3}\pi R^3}{8R^3} = \dfrac{\pi}{6} = 0.52$



b) Number of atoms of 1st nearest neighbors

- As you can see in the diagram, each atom has $c_1 = 6$ nearest neighbors ✓



- reference
- 1st nearest neighbors

c) Distance of 1st nearest neighbors.

- In SC structure, each atom and 1st nearest neighbors are at a distance of $d_{c_1} = a$. ✓

SEOUL NATIONAL UNIVERSITY
1 GWANAK-RO, GWANAK-GU, SEOUL, 08826, KOREA

3. Calculate the same properties (in Prob #2) for BCC structure with single type of atom (C, carbon) and conventional lattice parameter $a = 3.5$ Å (10 pt)

a) packing density

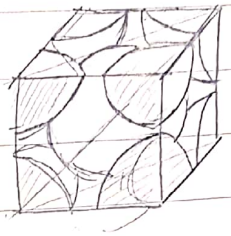
- Packing density $= \frac{n \times V_{sphere}}{V_{unit\ cell}}$, $n = \frac{1}{8} \times 8 + 1 = 2$
- $V_{unit\ cell} = a^3 = \frac{64}{3\sqrt{3}} R^3$

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

- $V_{sphere} = \frac{4}{3} \pi R^3$

$\therefore$ packing density $= \frac{2 \times \frac{4}{3} \pi R^3}{8 \times \frac{64}{3\sqrt{3}} R^3} = \frac{\sqrt{3}\pi}{8} = 0.68$

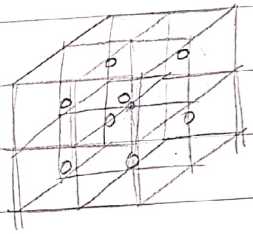
-3



b) Number of atoms of 1st nearest neighbors

- As you can see in the diagram, each atom has $CN = 8$ nearest neighbors which are located in the center of unit cells

✓



• reference
○ 1st nearest neighbors

c) Distance of 1st nearest neighbors.

- In BCC structure, each atom and 1st nearest neighbors are at a distance of $d_1 = 2R = \frac{\sqrt{3}}{2} a = 0.87a$

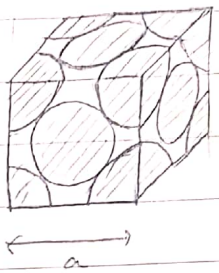
✓

4. Calculate the same properties (in Prob. #2) for fcc structure with single type of atom (C, carbon) and conventional lattice parameter $a = 3.5\,\text{Å}$ (10pt)

a) packing density of Fcc

- packing density $= \frac{n \cdot V_{sphere}}{V_{unit\ cell}}$, $n = \frac{1}{2}\times 6 + \frac{1}{8}\times 8 = 4$
- $V_{unit\ cell} = a^3$, $4R = \sqrt{2}a$ $\therefore V_{unitcell} = (2\sqrt{2})^3 R^3$
- $V_{sphere} = \frac{4}{3}\pi R^3$

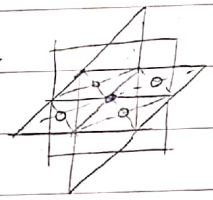
$\therefore$ packing density $= \frac{4 \times \frac{4}{3}\pi R^3}{(2\sqrt{2})^3 R^3} = 0.74$ ✓



3.

b) Number of atoms of 1st nearest neighbors.

- As you can see in the diagram, there are 4 nearest neighbors lying in a plane and there are 3 perpendicular plane including reference point, thereby $\underline{C_1 = 12}$ nearest neighbors ✓



- reference
- 1st nearest neighbors.

c) Distance of 1st nearest neighbors.

- In FCC structure, each atom and 1st nearest neighbors are at a distance of $d_{C_1} = 2R = \frac{\sqrt{2}}{2}a = \underline{0.71}\,a$ ✓

5. Portlandite [$Ca(OH)_2$] is a minor phase produced from cement hydration but it is important due to its impact on a pH of pore-solution. (50 pt, each 10 pt)

Its lattice parameters of portlandite are

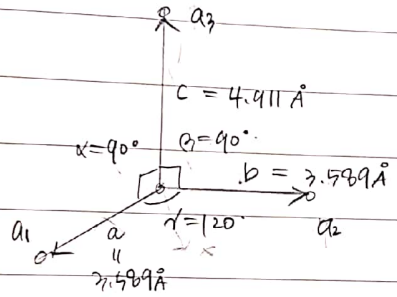
$a = 3.58900$; $b = 3.58900$) $c = 4.91100$ Å

$\alpha = 90.0$; $\beta = 90.0$; $\gamma = 120.0$ °

Based on the definition system, we can understand its Bravais crystal system is "Trigonal"

a) Define three lattice vectors from the given six lattice parameters.

From the given parameters, we can draw the below diagram, and



and three lattice vectors are

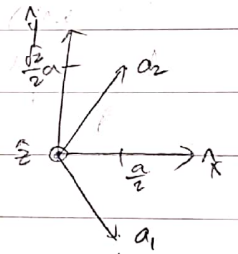
$a_1 = \frac{a}{2}\hat{x} - \frac{\sqrt{3}}{2}a\hat{y}$ (since $a=b$)

$a_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$

$a_3 = c\hat{z}$

then, $V_{cell} = \left(\frac{\sqrt{3}}{2}\right)a^2c$

($a=3.589$, $c=4.911$)



b) Fill the empty areas in Orthogonal Coordinates. Note that there is no single correct answer for this question.

① $H = 0.3334X + 0.6667Y + 0.5144Z$

$= \left(\frac{a}{2}\hat{x} - \frac{\sqrt{3}}{2}a\hat{y}\right) \times 0.3334 + \left(\frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}\right) \times 0.6667 + c\hat{z} \cdot X0.5144$

$= 3.589 \times \frac{1.0001}{2}\hat{x} + 3.589 \times \frac{0.3333\sqrt{3}}{2}\hat{y} + 4.911 \times 0.5144\hat{z}$

$= \underline{1.795}\hat{x} + \underline{1.036}\hat{y} + \underline{2.821}\hat{z}$ [Å]

② $H = 0.6667X + 0.3334Y + 0.4256Z$

$= \left(\frac{a}{2}\hat{x} - \frac{\sqrt{3}}{2}a\hat{y}\right) \times 0.6667 + \left(\frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}\right) \times 0.3334 + c\hat{z} \times 0.4256$

$= \underline{1.795}\hat{x} - \underline{1.036}\hat{y} + \underline{2.090}\hat{z}$ [Å]

③ $O = 0.3334X + 0.6667Y + 0.7663Z$

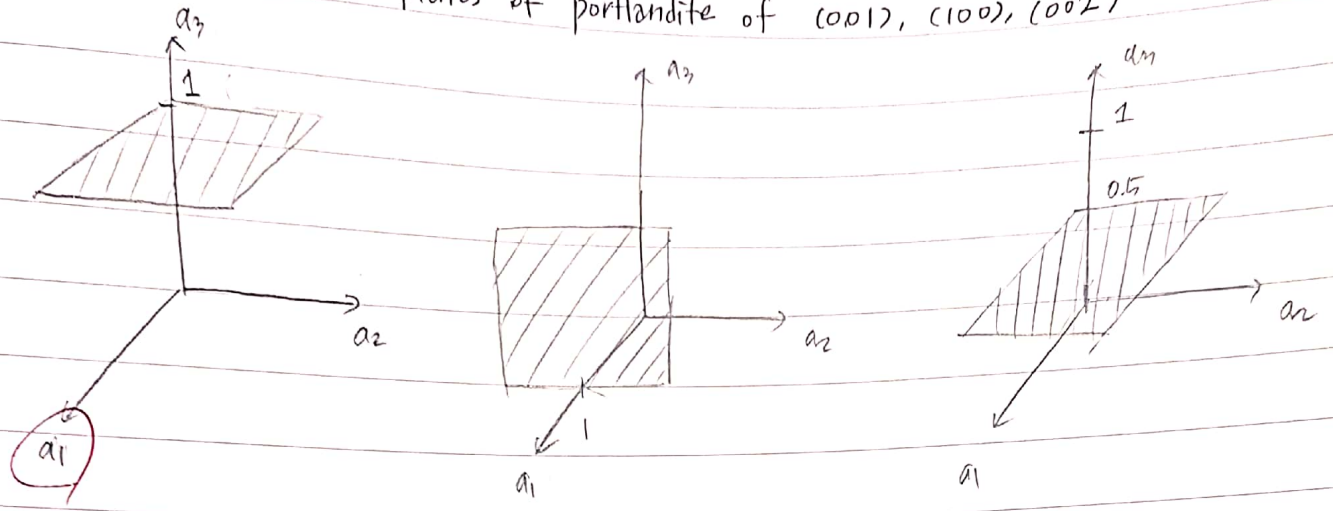
$= \underline{1.795}\hat{x} + \underline{1.036}\hat{y} + \underline{3.763}\hat{z}$ [Å]

④ $O = 0.6667X + 0.3334Y + 0.2331Z$

$= \underline{1.795}\hat{x} - \underline{1.036}\hat{y} + \underline{1.148}\hat{z}$ [Å]

MooKeuk

c) Sketch the (hkl) planes of portlandite of (001), (100), (002)

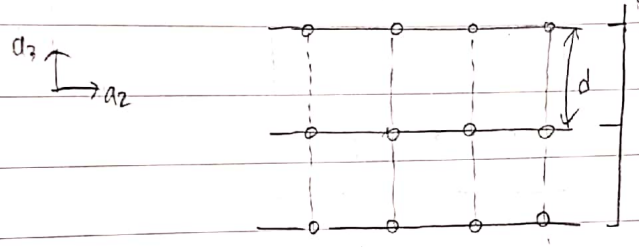


(001) plane ✓ (100) plane ✓ (002) plane ✓

d) what is the spacing of {001}?

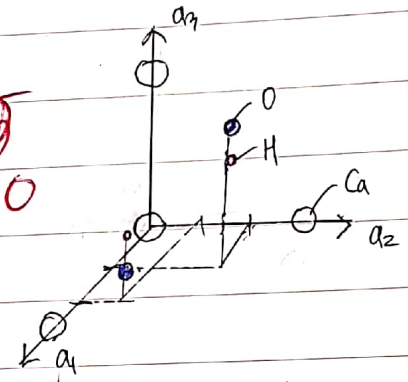
{001} planes

o : Ca



C = 4.911 Å

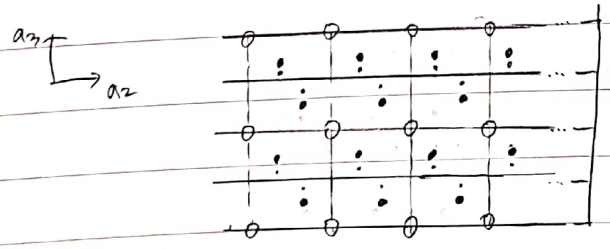
-1 10



e) will portlandite have (002) XRD peak? In other word, does portlandite have periodic arrangement of atoms in the position of (002) plane?

- To begin with, (002) peak appears in XRD pattern of portlandite. which has lower intensity than (001) peak.

{002} planes → Ca 원자가 한 평면 같이 평면에 나타난다



o : Ca

• : O

• : H

Most atomically crowded plane, which is (001), will provide relatively more intensity than (002) plane.

-5