

Advanced Construction Materials

Homework #1

Due: Mar 26th at 6pm.

1. (Self-study question) Explain different types bonding of Hydrogen Bond, Ionic Bond, Covalent Bond, and Metallic Bond **(20pt)**
2. For simple cubic structure with single type of atom (C, carbon) and lattice parameter $a = 3.5 \text{ \AA}$, calculate below properties: **(10pt)**
 - 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
3. Calculate the same properties (in Prob. #2) for BCC structure with single type of atom (C, carbon) and "conventional lattice parameter $a = 3.5 \text{ \AA}$ **(10pt)**
4. Calculate the same properties (in Prob. #2) for FCC structure with single type of atom (C, carbon) and "conventional lattice parameter $a = 3.5 \text{ \AA}$ **(10pt)**

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

Its lattice parameters of portlandite are

$$\mathbf{a} = 3.58900; \quad \mathbf{b} = 3.58900; \quad \mathbf{c} = 4.91100 \text{ \AA}$$

$$\mathbf{\alpha} = 90.0000; \quad \mathbf{\beta} = 90.0000; \quad \mathbf{\gamma} = 120.0000 \text{ deg}$$

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.

Below table contains basis vectors for each basis atoms defined in the crystal system of Trigonal. Portlandite consists of five basis atoms (or vectors). Fractional coordinates indicate each partial coordination defined in above three lattice vectors. Orthogonal coordinates were position of atoms in conventional orthonormal X, Y, and Z coordination system.

- b) Fill the empty areas in Orthogonal Coordinates. Note that there is no single correct answers for this question. Right answers can vary.

	Fractional Coordinates			Orthogonal Coordinates [\AA]		
	X	Y	Z	X_ortho	Y_ortho	Z_ortho
Ca	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H	0.3334	0.6667	0.5744			
H	0.6667	0.3334	0.4256			
O	0.3334	0.6667	0.7663			
O	0.6667	0.3334	0.2337			

- c) Sketch the (hkl) planes of portlandite of (001), (100), and (002)
- d) What is the spacing of $\{001\}$?
- e) Will portlandite have (002) XRD peak? In other word, does portlandite have periodic arrangement of atoms in the position of (002) plane?