

#### UNIVERSITY OF GHANA

(All rights reserved)

### **FACULTY OF ENGINEERING SCIENCES**

# BSc. (ENG) MATERIALS SCIENCE AND ENGINEERING

#### **END OF SECOND SEMESTER EXAMINATIONS: 2013/2014**

## MTEN 312: CRYSTAL CHEMISTRY OF CERAMICS (3 CREDITS)

TIME ALLOWED: TWO and HALF  $(2\frac{1}{2})$  HOURS

### Answer ALL Questions

## Question 1

- a) By considering the hybridization of orbitals in diamond explain why it is
  - (i) an electrical insulator at room temperature and
  - (ii) extremely hard.
- b) Explain why covalently bonded materials are generally less dense than ionically or metallically bonded ones.
- c) Sketch bond-energy curves for two ceramics, one with a high Young's modulus and one with a low Young's modulus.
- d) Rank the following ceramics in terms of decreasing fraction of ionic character in their bonds: SiC, AlN, Si<sub>3</sub>N<sub>4</sub>, B<sub>4</sub>C, GaN, Al<sub>2</sub>O<sub>3</sub>, and SiO<sub>2</sub>. **Table 1** is the electronegativity differences for the various ceramics.

Table 1. Electronegativity differences for the various ceramics

SiC	AlN	Si <sub>3</sub> N <sub>4</sub>	B <sub>4</sub> C	GaN	Al <sub>2</sub> O <sub>3</sub>	SiO <sub>2</sub>
0.7	1.5	1.2	0.5	1.5	0.5	0.2

15 Marks

#### Question 2

- a) What is the difference between atomic structure and crystal structure?
- b) Figure 1 has two different crystal packings; (i) for a non-dense or random packing and (ii) is for dense packing. Sketch graphically their energy (E) versus their interparticles distances (r) and comment on these two parameters with respect to the structural packing in (i) and (ii).

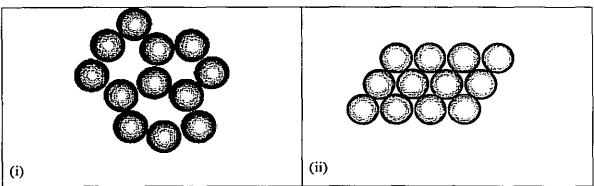


Figure 1. Two different crystal packings for (i) non-dense and (ii) dense

- c) Prove that the atomic packing factor (APF) for Gallium Arsenide (GaAs) is 0.41. The atomic radii for (Ga) and (As) are 0.135 and 0.125 nm, respectively. The lattice parameter is 0.565 nm.
- d) Does rutile structure obey Pauling's rules?
- e) Sketch the lattice structure of Kaolinite and Montmorillonite minerals. What separates the lattice structure of a Montmorillonite mineral from that of Mica?

17 Marks

### Question 3

- a) Show that, for the body-centered cubic crystal structure the unit cell edge length "a", and the atomic radius "R", are related by,  $a = 4R / \sqrt{3}$ .
- b) For the hexagonal close pack (HCP) crystal structure, show that the ideal ratio c/a is 1.633.
- c) Assuming a cubic crystal system, make a sketch of the following planes (001), (111), (123),  $(\overline{1}10)$ , (010),  $(\overline{1}\overline{1}\overline{1})$ ,  $(0\overline{1}0)$ .
- d) What information is needed to specify a crystal structure?
- e) The unit cell for Tin has tetragonal symmetry, with 'a' and 'b' lattice parameters of 0.583 and 0.318 nm, respectively. If its density, atomic weight, and atomic radius are 7.27 g/cm<sup>3</sup>, 118.71 g/mol, and 0.151 nm, respectively, compute the atomic packing factor.

[Avogadro's number =  $6.022 \times 10^{23}$  atoms/mol]

18 Marks

# Question 4

a) Write out the symmetry elements present in the 'molecules' in **Figure 2** and the corresponding point group of each one. Assume that the molecules are planar, exactly as drawn, and not three-dimensional. The shapes are: (i) pentagonal C<sub>5</sub>H<sub>5</sub>, in ferrocene; (ii) linear, CS<sub>2</sub>; (iii) triangular, SO<sub>2</sub>; (iv) square, XeF<sub>4</sub>.

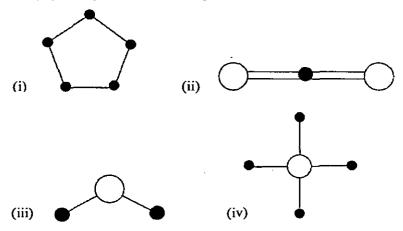


Figure 2. Molecular structures for (i) C<sub>5</sub>H<sub>5</sub> (ii) CS<sub>2</sub> (iii) SO<sub>4</sub> and (iv) XeF<sub>4</sub>

- b) The metal iridium has an FCC crystal structure. If the angle of diffraction for the (220) set of planes occurs at 69.22° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1542 nm is used, compute;
  - (i) Interplanar spacing for this set of planes and
  - (ii) Atomic radius for an iridium atom.
- c) An x-ray diffraction pattern for α-iron taken using a diffractometer and monochromatic x-radiation having a wavelength of 0.1542 nm is shown in Figure 3; each diffraction peak on the pattern has been indexed. Compute the interplanar spacing for each set of planes indexed; also determine the lattice parameter of Fe for each of the peaks.

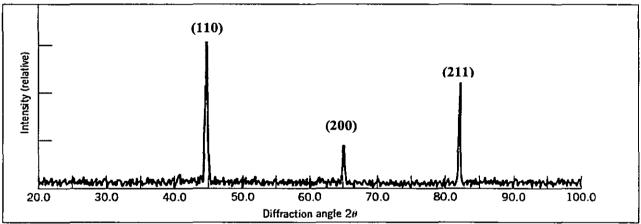


Figure 3. X-ray diffraction pattern for α-iron

20 Marks