

**Final Exam. "Diffraction rays & its applications" (352 P)**

May: 2018

Time: 3 hours

**Answer only Five Questions:**

- 1.a) Show a schematic diagram of an experimental tools of the produced XRD for determining the crystal structure of a single crystal
- b) X-ray beam incident on (100) plane of FCC structure , Prove that the energy of the beam is related to the diameter of the crystal (A) and the Bragg's angle for 2<sup>nd</sup> reflection( $\theta$ ) as:  $E(kev) = C(A \sin \theta)$ , calculate the constant C.
- 2.a) Prove that: (i) The packing factor of BCC is less than that for FCC, (ii) for a simple cubic lattice:  $d_{110} : d_{111} = \sqrt{3} : \sqrt{2}$
- b) Explain the graphical representation of Bragg's law in terms of reciprocal lattice vector ( $G_{hkl}$ ).
- 3.a) If the momentum and energy of the electron is related by:  $P = (2m_0 E + \frac{E^2}{C^2})^{1/2}$  find the corresponding relativistic increase of the mass in terms of the high accelerating voltage.
- b) Find the density ratio of a certain material having BCC, and FCC structures at different temperatures.
- 4.a) Explain one of the X-ray spectrum resulting in the pattern of X-ray diffraction. Show the parameter that depends  $\lambda$ .
- b) A certain crystal reflect monochromatic X-rays strongly when Bragg's angle of the 3<sup>d</sup> order is  $51^\circ$ , satisfy the Bragg's reflection for the first and second order spectrum. If the wavelength having the same order of magnitude of the lattice parameter of the crystal calculate the Bragg's angle reflected at (010) – plane.
- 5.a) Prove that the modification of Bragg's law for the higher reflection order  $n$  can be expressed in the form:  $n\lambda = 2d \sin \theta [1 - (1 - \delta) / \sin^2 \theta]^{1/2}$ , determine the parameter  $\delta$  as a function of the refractive index.
- b) Consider a BCC crystal of atomic radius  $0.466 \text{ \AA}$ , determine the energy of X-ray beam incident on (111) plane with angle  $8.8^\circ$  for 1<sup>st</sup> order spectrum ( $h = 6.62 \times 10^{-27} \text{ erg. sec.}$ ).
- 6.a) Draw a schematic diagram of an experiment for measuring the wavelength of the electron-diffraction, find an expression of the diffraction diameter in terms of the d-spacing and accelerating high voltage.
- b) X-ray beam with energy 2.7 KeV incident on BCC crystal with angle  $30^\circ$ , determine the crystalline plane reflected the 1<sup>st</sup> order spectrum (given: atomic radius of 0.2 nm, and  $h = 6.62 \times 10^{-27} \text{ erg. sec.}$ )

انتهت الأسئلة

تمنياتي بالتوفيق والتفوق ..... ا.د. عبد المنعم سلطان .....



Faculty of Science  
Physics Department

Date: 29 May, 2018  
Time: 3 hours

Final Examination in (X-ray Diffraction & Applications 352P)

Teaching Staff: Prof. Dr. Abdulaziz Abualfadi

**Constants:**  $h = 6.626 \times 10^{-34} \text{ J.s}$ ,  $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$ ,  $k_B = 1.38 \times 10^{-23} \text{ J/K}$ ,  $e = 1.6 \times 10^{-19} \text{ C}$ ,  
 $c = 3 \times 10^8 \text{ m/s}$ ,  $N_A = 6.02 \times 10^{23} \text{ atom/mole}$ ,  $m_e = 9.1 \times 10^{-31} \text{ kg}$ ,  $m_n = 1.67 \times 10^{-27} \text{ kg}$

**Answer 5 questions from the following: [10 marks for each]**

1- (a): How the laue technique particularly convenient for checking the orientation of crystals. Show why laue method cannot be used for crystal structure determination.

(b): Calculate the three smallest Bragg angles that arise from the diffraction of 100 keV electrons in copper with lattice parameter at room temperature equal  $3.615 \text{ \AA}$ ?

2- (a)- Why X-rays are used for diffraction studies in crystals. Write a note on neutron diffraction.

(b)- Sodium crystallizes in a cubic lattice with lattice constant  $4.3 \text{ \AA}$ . The density of sodium is  $963 \text{ kg/m}^3$  and its atomic weight is  $23 \text{ g/mole}$ . How many atoms are contained in one unit cell? What type of cubic unit cell does sodium form?

(c)- A neutron beam with energies of  $15 \times 10^6 \text{ eV}$ . The beam is incident on a single crystal of aluminum with lattice constant  $404.95 \text{ pm}$  along  $[100]$  direction. In which direction is the beam scattered?

3- (a)- Show the technique of X-ray structure determination in which a single crystal specimen is rotated in a beam of monochromatic X-rays.

(b)- Determine unit cell dimension when Bragg's angle of  $45^\circ$  is observed during first order reflection in a cubic crystal having Miller indices  $(100)$ . Given the wavelength of the X-ray used is  $2 \text{ \AA}$ .

4- (a)- Find the atomic packing factor for face centered cubic (F.C.C) crystal.

(b)- The spacing of the paned of a crystal is  $1.2 \text{ \AA}$  and the angle for the first order reflection is  $30^\circ$ . Determine the energy of the X-rays in eV.

5- (a)- Discuss in brief the factors affecting X-ray spectrum.

(b)-Find the geometrical structure factor ( $F_{hkl}$ ) for body centered cubic (B.C.C) by taking the cell contain one eighth of an atom at each of its eight corners, plus one atom at the center.

6- (a) What is the meaning of the crystallographic symbols:  $m$ ,  $\bar{3}$ ,  $4/m$ ,  $4$ ,  $X$ ,  $X/\text{mm}$ , and show the equivalence of  $\bar{2}$ .

(b)-. Explain and derives Bragg's law of X-ray diffraction from a crystal. Then draw the  $[101]$ ,  $[120]$  and  $[121]$  directions within a cubic unit cell and sketch the planes  $(112)$  and  $(110)$ .

انتهت الأسئلة مع أطيب الأمنيات بالتوفيق



**Part II: Solve ONLY FIVE problems from the following: (30 Marks)**

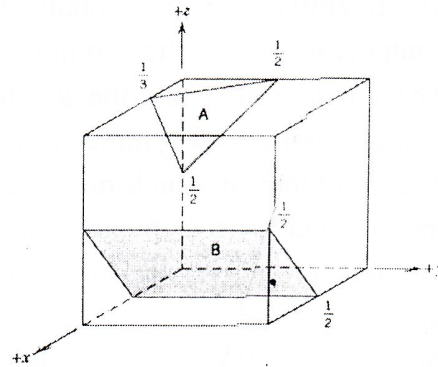
1. Zirconium (Zr) has an HCP crystal structure and a density of  $6.51 \text{ g/cm}^3$ .

(a) What is the volume of its unit cell in cubic meters?

(b) If the  $c/a$  ratio is 1.593, compute the values of  $c$  and  $a$ .

[Hint:  $A_{\text{Zr}} = 91.22 \text{ g/mol}$ ]

2. Determine the Miller indices for the planes (A & B) shown in the following unit cell:



3. For which set of crystallographic planes will a first-order diffraction peak occur at a diffraction angle of  $2\theta = 46.21^\circ$  for BCC iron when monochromatic radiation having a wavelength of  $0.0711 \text{ nm}$  is used? [Hint: atomic radius of iron =  $0.1241 \text{ nm}$ ].

4. Calculate the activation energy (in eV) for vacancy formation in aluminum, given that the equilibrium number of vacancies at  $500^\circ\text{C}$  is  $7.57 \times 10^{23} \text{ m}^{-3}$ . The atomic weight and density (at  $500^\circ\text{C}$ ) for aluminum are  $26.97 \text{ g/mol}$  and  $2.62 \text{ g/cm}^3$ , respectively.

5. Calculate the unit cell edge length for an 85 wt% Fe-15 wt% V alloy. All of the vanadium is in solid solution, and, at room temperature the crystal structure for this alloy is BCC. The atomic weights for Fe and V are  $55.8$  and  $50.94 \text{ g/mol}$ , whereas the densities for the Fe and V are  $7.87 \text{ g/cm}^3$  and  $6.10 \text{ g/cm}^3$ , respectively.

6. Iron (Fe) and vanadium (V) both have the BCC crystal structure and V forms a substitutional solid solution in Fe for concentrations up to approximately 20 wt% V at room temperature. Determine the concentration in weight percent of V that must be added to Fe to yield a unit cell edge length of  $0.29 \text{ nm}$ .

Best Wishes

Constants:  $N_A = 6.022 \times 10^{23} \text{ atoms/mol}$ ;  $k_B = 1.38 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-1} \text{ K}^{-1}$



**Part I: Answer all the following questions:**

**(20 Marks)**

**(A): Put (✓) or (×) for all the following sentences:**

**(5 Marks)**

1. Crystal structure = base + lattice ( ).
2. The primitive unit cell contains the same kind of atoms, while the Bravais lattice contains only one lattice point ( ).
3. The cubic system has the greatest degree of symmetry, but the orthorhombic system has the least symmetry ( ).
4. The substance in which measured properties are independent of the direction of measurement is isotropic material ( ).
5. Precipitates are classified as volume defect while vacancies classified as a linear defect ( ).
6. Schottky is equivalent to missing atom that leaves its original site and migrates to another position in the crystal ( ).
7. A screw dislocation being formed by a shear stress that is applied to produce the distortion ( ).
8. Both of dislocation and external surfaces can be classified as two-dimensional imperfection ( ).
9. Coordination number in body-centered cubic crystal structure is 12 ( ).
10. Point defects are thermodynamically stable defects ( ).

**(B) Give reason(s) for the following:**

**(5 Marks)**

1. X-ray can be used to detect the crystallinity of materials.
2. The atomic packing factor always less than 1.
3. The physical properties of single crystals of some substances depend on the crystallographic direction in which measurements are taken.
4. For some elements, the degree of dissolvability of the solute (minor) and solvent (major) atoms is low.
5. There is no ideal crystal in nature.

**(C) Write in details on the following:**

**(10 Marks)**

1. Intercept method for the grain size determination.
2. Single crystal and polycrystalline structures.
3. Surface defects and volume defects.
4. Electron microscopes.



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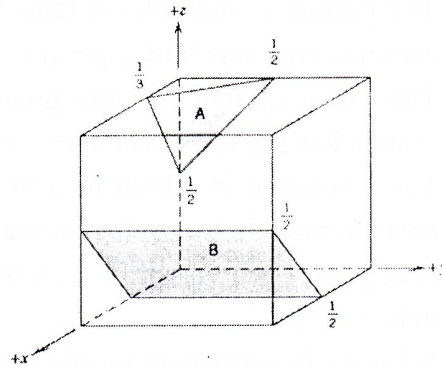
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Best Wishes

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Faculty of Science  
Physics Department

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Teaching Staff: Prof. Dr. Abdulaziz Abualfadi

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