National Exams December 2016

98-Phys-B7, Structure of Materials

3 Hours Duration

NOTES:

1. Attempt any **five** questions out of **seven**. **Only the first five** questions as they appear in your answer book will be marked.

2. All questions carry equal weightage (20 marks).

3. Candidates may use one of two calculators, the Casio or Sharp approved models. This is a CLOSED BOOK exam. All necessary equations, constants and diagrams are provided in the appendix.

4. If a doubt exists as to the interpretation of any question, equation or data given, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made.

Question I: Electron Structure

1. **(6 marks)** Brief explain, with an example, the following concepts regarding the atomic structure of materials:
   a. Aufbau principle
   b. Pauli's exclusion principle
   c. Electronegativity

2. **(4 marks)** Calculate the energy change when an electron in a hydrogen atom undergoes a transition from n=4 to n=3 state. Is the energy absorbed or emitted?

3. **(10 marks)**
   a. **(2+2 = 4 marks)** Compute the electromagnetic energy emitted by a single quantum when a tungsten filament is heated, given that the frequency of radiation is 1 Hz. What is the wavelength of the radiation emitted?
   b. **(2+4 = 6 marks)** What is the de Broglie's hypothesis? Calculate the uncertainty associated with speed of an electron moving at $1/6^{th}$ the speed of light, if the uncertainty in knowing its position is one percent.

Question II: Bonding

1. **(10 marks)** Suppose the net potential energy between two atoms is given by: $E = -\frac{A}{r^m} + \frac{B}{r^n}$, where r is the interatomic spacing and A and B are constants. Derive an expression for force, F, vs. interatomic spacing; and evaluate the equilibrium interatomic spacing and the maximum binding energy. Qualitatively draw the plots of E vs. r and F vs. r, while indicating important points on the plots.

2. **(5 marks)** Identify the dominant type of bonding in the following materials:
   (a) Si, (b) Graphite, (c) NaCl, (d) SiO_2, (e) Zr.

3. **(5 marks)** What are the four quantum numbers required to uniquely express a given electron state? Give one possible combination of the four quantum numbers which would describe the state of valence electron in Br^{-1} (Z=35).

Question III: Crystal Structure I

1. **(6 marks)** Determine the density of BCC iron, which has a lattice parameter of 0.2866 nm, given its molar mass is equal to 55.847 g/mol.

2. **(6 marks)** Calculate the ideal packing factor for HCP lattice, with $c/a = 1.633$.

3. **(8 marks)** Draw the following planes and directions (use separate drawings).
   (a) Planes in cubic unit cells: $(1\bar{1}0)$, (221)
   (b) Directions in hexagonal unit cells: $[1\bar{1}00]$, $[11\bar{2}0]$

Question IV: Crystal Structure II

1. **(6 marks)** The density of vanadium (Z=23) is 5.8 g/cm^3. Determine whether it has a face centered cubic or body centered cubic crystal structure. It is provided that the unit cell length is 0.303 nm and the molar mass is 50.94 g/mol.

2. **(6 marks)** Explain the factors that govern solubility of one element in another. Using the data provided below, predict the relative degree of solubility of zinc and lead in copper.

Element	Atom radius (nm)	Crystal structure	Electronegativity	Valence
Copper	0.128	FCC	1.8	+2
Zinc	0.133	HCP	1.7	+2
Lead	0.175	FCC	1.6	+2, +4

3. **(8 marks)** Calculate the equilibrium number of vacancies per cubic meter of magnesium at 700°C if the activation energy for vacancy formation is 0.8 eV, the molar mass for Mg is 24.304 g/mol, and its density is 1.74 g/cm^3.

Question V: Microstructural Characterization

1. **(10 marks)** The X-ray diffraction of a sample of BCC iron contains a peak occurring at 2θ = 44.704° for {110} planes. Calculate the lattice constant of the material if the wavelength of the incoming ray was 0.1541 nm. At what angle of incidence will the diffraction peak for {211} planes occur?

2. **(10 marks)** Compare scanning electron microscopy and transmission electron microscopy in terms of: (a) physical principle, (b) typical range of energies at which electrons are energized, (c) resolution and magnification, and (d) ability to produce a three dimensional image. Which of these can reveal details on sub-surface dislocation activity in a metallic thin sample?

Question VI: Dislocation Theory and Grain Boundaries

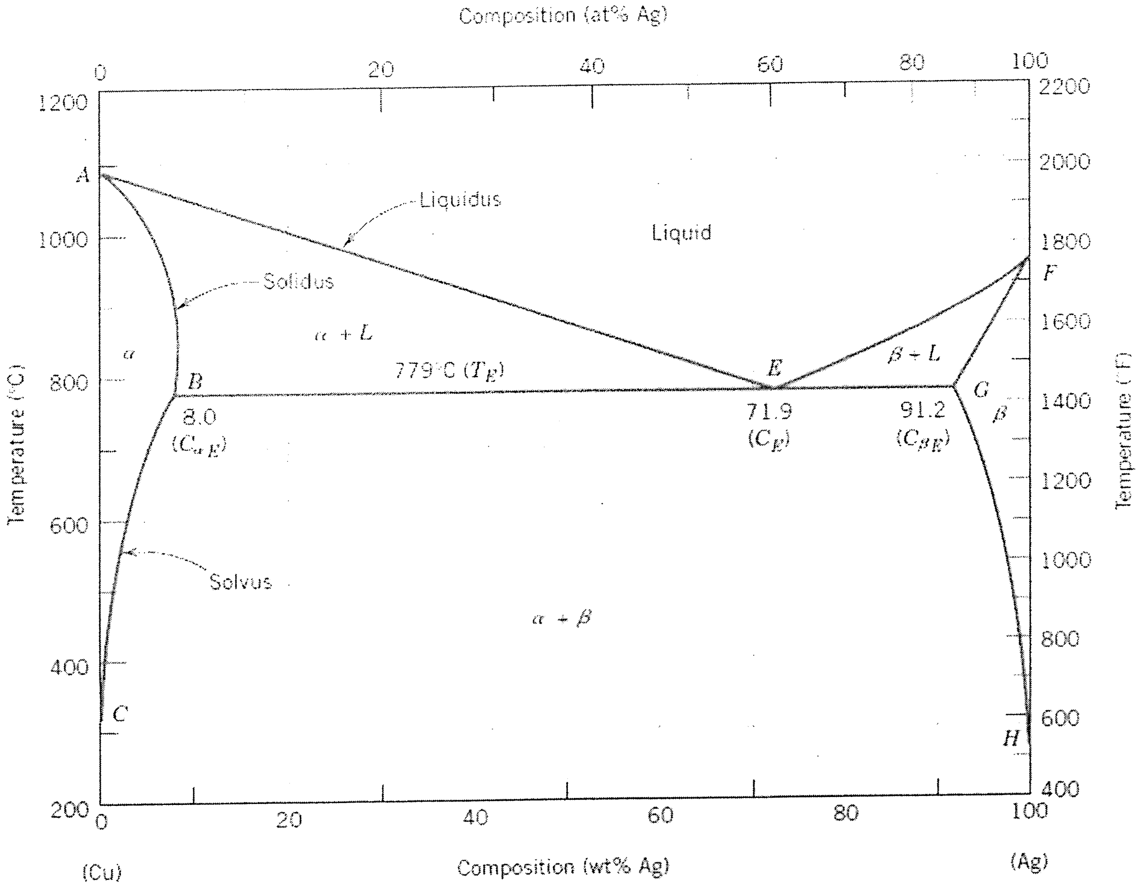
1. **(6 marks)** What is the Schmid law? Applying this concept, determine if the slip will occur when a single crystal is oriented such that the slip plane is normal to the applied tensile stress.

2. **(6 marks)** Write down the main slip systems for HCP lattice.

3. **(8 marks)** During strain hardening, the density of dislocations in the material rises. The critical resolved shear stress (CRSS) can be expressed as a function of dislocation density by $\tau_{crss} = \tau_0 + \alpha G b \sqrt{\rho}$ where τ_0 is the intrinsic strength, α is a material constant, G is the shear modulus, b is the Burgers vector, and ρ is the dislocation density per unit area. For a copper polycrystal, determine the following:
   a. Determine the Burgers vector of an edge dislocation in the slip plane and its magnitude if the lattice constant of copper is 3.615 Å. **(3 marks)**
   b. **(5 marks)** If CRSS is equal to 2.10 MPa at a dislocation density of 10^5 /mm^2, determine the value of τ_{crss} at a dislocation density of 10^7 /mm^2. The shear modulus is 48 GPa and α =0.2.

Question VII: Phase Diagram

(**20 marks**) For the binary eutectic phase diagram for copper-silver (Cu-Ag) shown below, answer the following questions: (**4 parts of 5 marks each=20 marks**)



1. For a 40 wt% Cu-60wt%Ag alloy at a temperature of 800°C, what phases are present in the system and what are their compositions?
2. At 700°C, what is the maximum solubility of: (a) Cu in Ag? (b) Ag in Cu?
3. Define eutectic reaction. Write eutectic reaction for the Cu-Ag system.
4. Determine the relative mass fractions of the phases present in a 55wt%Ag-45wt%Cu alloy at 800°C.

Appendix: Equations and constants

Avogadro's number = 6.023×10^{23} molecules/mol　　Universal gas constant (R) = 8.31 J/mol-K

Boltzmann's constant (k) = 1.38×10^{-23} J/atom-K = 8.62×10^{-5} eV/atom-K　　1 eV = 1.6022×10^{-19} J

Planck's constant, $h = 6.63 \times 10^{-34}$ J.s　　Electron mass, $m_e = 9.11 \times 10^{-31}$ kg

1 MPa = 10^6 N/m^2　　1 GPa = 10^9 N/m^2

$$n = 1,2,3,\ldots \qquad l = 0,1,2,\ldots n-1 \qquad m_l = 0,\pm1,\pm2,\pm3,\ldots\ldots\pm l \qquad m_s = \pm 1/2$$

$$F = -\frac{\partial E}{\partial r} \qquad E_n = -\frac{Z^2 R_E}{n^2} \qquad \Delta E = E_i - E_f = R_E\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \qquad R_E = 13.61\,\text{eV}$$

$$E = h\nu \qquad \nu\lambda = c \qquad \lambda = \frac{h}{mv} \qquad \Delta x.\Delta p \geq \frac{h}{4\pi}$$

$$N_D = N\exp\left(-\frac{Q_D}{kT}\right) \qquad N = \frac{\rho N_A}{A_{wt}};\ A_{wt} = \text{atomic weight} \qquad T_K = T_C + 273;\ A = \pi r^2;\ \ V = \frac{4}{3}\pi R^3$$

$$a = 2R \qquad a = 2\sqrt{2}R \qquad a = \frac{4}{\sqrt{3}}R \qquad APF = \frac{V_s}{V_c} \qquad \rho = \frac{n.A_{wt}}{V_c.N_A}$$

$$n\lambda = 2d\sin\theta \qquad \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}; \qquad \text{if } a = b = c, \text{ then } d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$J_x = -D\frac{\partial c}{\partial x} \qquad \frac{\partial c_x}{\partial t} = D\frac{\partial^2 c_x}{\partial x^2} \qquad \frac{C_s - C_x}{C_s - C_0} = erf\left(\frac{x}{2\sqrt{Dt}}\right) \qquad D = D_0\exp\left(-\frac{Q_d}{RT}\right)$$

$$\tau_R = \sigma.\cos\phi.\cos\lambda \qquad \sigma = \sigma_0 + k.d^{-1/2} \qquad \varepsilon = \frac{\Delta l}{l_0} \qquad \sigma = \frac{F}{A_0} \qquad \sigma = E\varepsilon \qquad \tau = \frac{F}{A_0}\ \ \tau = G\gamma$$

$$E = 2G(1+\upsilon) \qquad \nu = -\frac{\varepsilon_y}{\varepsilon_x} \qquad \%EL = 100\,\varepsilon_f$$

TABLE OF THE ERROR FUNCTION

z	erf(z)	z	erf(z)	z	erf(z)	z	erf(z)
0	0	0.40	0.4284	0.85	0.7707	1.6	0.9763
0.025	0.0282	0.45	0.4755	0.90	0.7970	1.7	0.9838
0.05	0.0564	0.50	0.5205	0.95	0.8209	1.8	0.9891
0.10	0.1125	0.55	0.5633	1.0	0.8427	1.9	0.9928
0.15	0.1680	0.60	0.6039	1.1	0.8802	2.0	0.9953
0.20	0.2227	0.65	0.6420	1.2	0.9103	2.2	0.9981
0.25	0.2763	0.70	0.6778	1.3	0.9340	2.4	0.9993
0.30	0.3286	0.75	0.7112	1.4	0.9523	2.6	0.9998
0.35	0.3794	0.80	0.7421	1.5	0.9661	2.8	0.9999