National Exams December 2017

10-Met-A4, 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**) Briefly explain, with an example and/or sketch, the following concepts regarding the atomic structure of materials:
   a. Wave-particle duality
   b. Hiesenberg uncertainty principle
   c. Hund's rule.

2. (**4 marks**) Explain, with pictorial representation, the key differences between Bohr's atomic model and quantum mechanical model. Which one is considered more accurate and why?

3. (**4 marks**) Sketch the curves for potential energy vs. atomic separation and interatomic force vs. atomic separation, clearly indicating equilibrium atomic separation and bond energy. Explain how the Young's modulus can be determined from these curves.

4. (**6 marks**) An energy of 419 kJ mol^{-1} is required to convert (in the gas phase) potassium atoms to potassium ions and electrons. Given that 1 kJ mol^{-1} equals 1.67×10^{-21} joule per atom, calculate the longest possible wave length of light which is capable of ionising potassium atoms.

Question II: Bonding

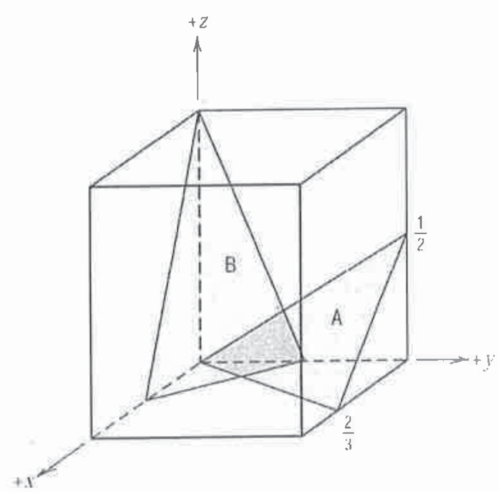
1. (**4 marks**) Briefly describe the four different types of bonding between atoms, ions or molecules in the solid state. What bond types do we find in the four broad categories of engineering materials (i.e. metals, ceramics, polymers, and semiconductors)?

2. (**4 marks**) Based on chemical bonding, explain why diamond is hard while graphite is soft. Identify and draw their crystal structure in your explanation. Also indicate different types of bonds in your drawings.

3. (**3*4 = 12 marks**) Write down the electronic configurations of individual ions in following compounds: (i) NaCl, and (ii) MgO.

Question III: Crystal Structure I

1. (**4 marks**) Determine the Miller indices for the planes shown in the adjacent unit cell. Clearly show your derivation steps.



2. (**6 marks**) Calculate the theoretical volume change if a pure metal undergoes a polymorphic transformation in from BCC to FCC crystal structure. Assume the hard-sphere atomic model and that there is no change in atomic volume before and after the transformation.

3. (**10 marks**) Cadmium telluride (CdTe) has the zinc blende crystal structure and a lattice parameter of 0.648 nm. Calculate the theoretical density of CdTe in g/cm^3. The molar masses for Cd and Te are 112.4 g/mol and 127.6 g/mol, respectively.

Question IV: Crystal Structure II

1. **(6 marks)** Explain why real crystals will always contain point defects. What is the effect of temperature on equilibrium density of point defects? If their equilibrium density at two different temperatures T_1 and T_2 is denoted by ρ_1 and ρ_2, respectively, then derive the relation for ρ_1/ρ_2.

2. **(6 marks)** What is the difference between interstitial and substitutional impurity defects? Explain using a schematic representation and provide at least one example of each.

3. **(8 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

Question V: Microstructural Characterization

1. **(20 marks)** Nickel is face centered cubic and has an atomic radius of $R = 0.125\ nm$.

a. **(12 marks)** Calculate the 2θ values for the first three diffraction peaks that would be obtained in an X-ray diffraction run for a nickel powder sample using Cu-K$_\alpha$ radiation ($\lambda = 0.1542\ nm$). First, calculate the lattice parameter. Then write down possible planes and apply the appropriate reflection rules. Now, calculate the interplanar spacing for these planes. Finally, calculate the 2θ values.

b. **(4 marks)** How would this answer change if the nickel sample is a single crystal with the (100) plane parallel to the surface?

c. **(4 marks)** Using XRD, how would you determine if a metal has FCC or BCC crystal structure?

Question VI: Diffusion and Grain Boundaries

1. **(8 marks)** Consider the gas carburising of a steel alloy at 950°C with an initial carbon concentration of 0.25 wt%. If the carbon concentration at the surface is suddenly brought to and maintained at 1.20 wt%, how long will it take to achieve a carbon content of 0.80 wt% at a position 0.5 mm below the surface? The diffusion coefficient for carbon in iron at this temperature is 1.6×10^{-11} m^2/s; and assume that the steel piece is semi-infinite.

2. **(6 marks)** Based on slip theory, explain which of FCC or HCP lattice is more ductile. Write down the main slip systems for these crystal structures.

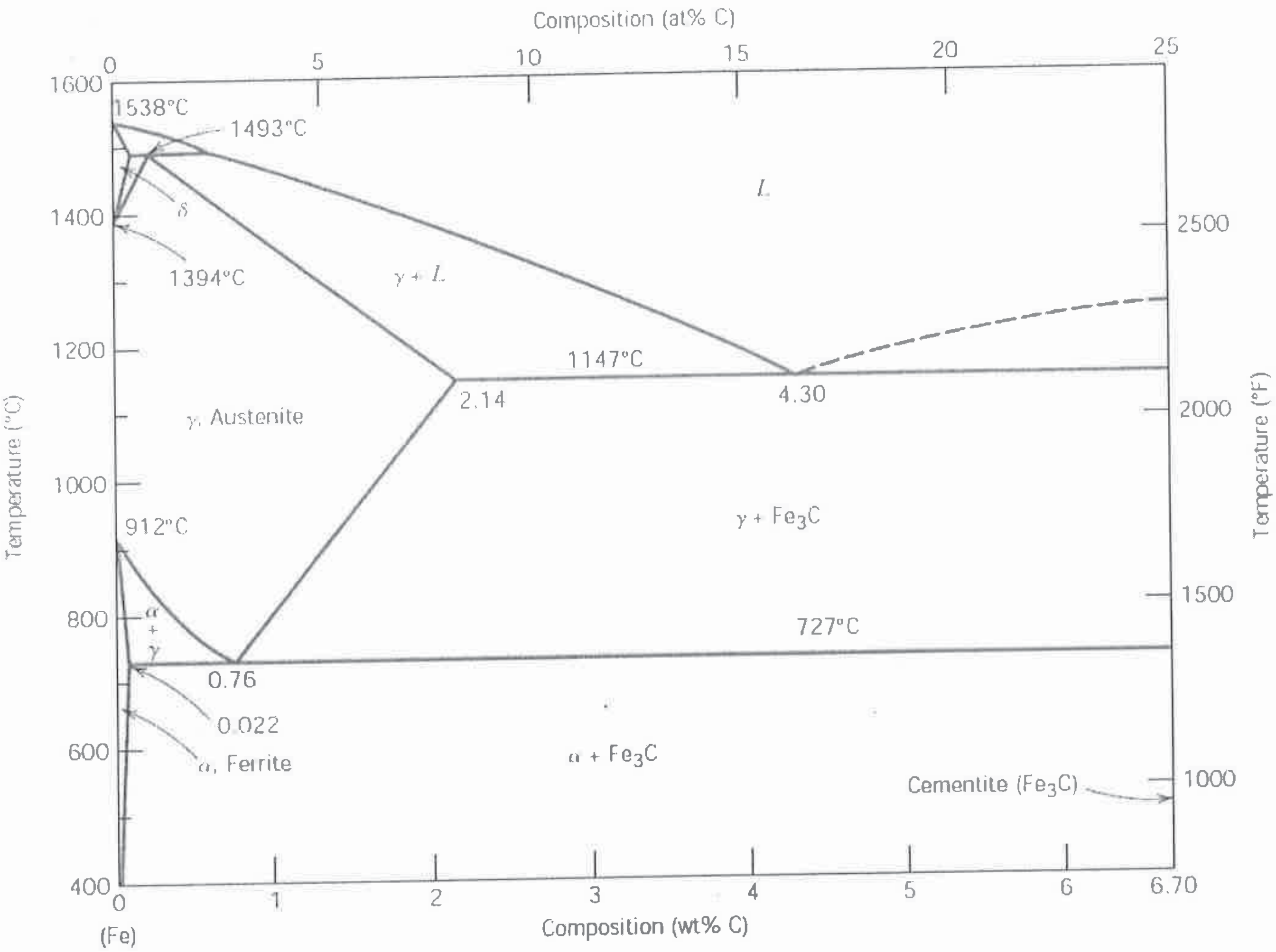
3. **(6 marks)** The relation between grain size (d) and yield strength of a metallic alloy can be expressed as $\sigma_y = \sigma_i + k_y d^{-\frac{1}{2}}$, where $\sigma_i = 3$ MPa is the friction stress, and $k_y = 0.5\ \text{MPa}.\text{m}^{\frac{1}{2}}$ is a constant. As received sample of this alloy has an average grain size of 4 μm. After annealing, the grain size increases to 104 μm.

a. **(3 marks)** Calculate the percentage decrease in yield strength of the alloy due to the annealing.

b. **(3 marks)** The grain growth during this process follows the relation $d^n - d_0^n = Kt$, where d_0 and d represent initial and final grain sizes for the process, t is time, and $n = 4$ and $K = 4.4\ \mu m^n s^{-1}$ are constants. Determine the time taken by the annealing process.

Question VII: Phase Diagram

(20 marks) For the binary eutectic phase diagram for iron-carbon (Fe-C) shown below, answer the following questions: **(5 parts of 4 marks each)**



1. What are the phases present at 2 wt% carbon content and a temperature of 1000°C?
2. Determine the maximum solubility of carbon in α-ferrite and austenite phases.
3. Explain the effect of increasing carbon content in iron on strength and ductility of the alloy system.
4. For a 99.65 wt% Fe-0.35 wt% C alloy at a temperature just below 727°C, determine the fractions of phases present.
5. Define eutectoid and eutectic reactions. Write down these reactions for the Fe-C system.

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

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

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

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

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

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

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

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

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

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

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