National Exams December 2018

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: Atomic Structure

1. (**2*3 = 6 marks**) Briefly explain, with an example and/or sketch, the following concepts regarding the atomic structure of materials:
   a. Bohr's atomic model vs. quantum mechanical atomic model,
   b. Aufbau principle,
   c. Transition metals.

2. (**2*3 = 6 marks**) Write down electronic structures of following ions:
   a. Co^{3+} (Z = 27), b. Cu^{2+} (Z = 29), c. Cl^- (Z=16)

3. (**8 marks**) Suppose the net potential energy between two atoms is given by:

$$E(r) = -\frac{1.436}{r} + \frac{7.32 \times 10^{-6}}{r^8}$$

   where r is the interatomic spacing. Determine the equilibrium interatomic spacing, r_0..

Question II: Chemical Bonding

1. (**4+2+2 = 8 marks**) Differentiate between metallic and van der Waals bonds. Give examples. Which of these has higher bonding energy? Which will correlate with a lower melting point?

2. (**6 marks**) Assuming that silica (SiO_2) has 100% covalent bonding, describe how oxygen and silicon atoms are joined in silica. Draw the full crystal structure in your explanation.

3. (**2*3 = 6 marks**) Identify the major type of bonding present in following materials:
   a. NaCl, b. CH_4, c. polymer chains.

Question III: Crystal Structure I

1. (**8 marks**) Draw the following crystal directions and planes in simple cubic and hexagonal cubic unit cells:
   a. [111], b. $[1\bar{2}10]$
   c. (132), d. $(2\bar{2}10)$

2. (**4 marks**) Explain the difference between stacking sequence for FCC and HCP materials.

3. (**8 marks**) Gallium Arsenide (GaAs) has the zinc blende crystal structure and a lattice parameter of 0.565 nm. Calculate its theoretical density in g/cm^3. The molar masses for Ga and As are 69.72 g/mol and 74.91 g/mol, respectively.

Question IV: Point Defects in Crystalline Solids

1. (**8 marks**) Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density at this temperature are given as 63.5 g/mol and 8.4 g/cm^3, respectively.
2. (**4 marks**) Differentiate between Frenkel and Schottky defects, with an example.
3. (**8 marks**) A niobium alloy is produced by introducing tungsten substitutional atoms into the BCC structure; eventually an alloy is produced that has a lattice parameter of 0.32554 nm and a density of 11.95 g/cm^3. Calculate the fraction of tungsten atoms in the alloy. The atomic weights and densities are given as 92.91 g/mol and 8.57 g/cm^3, respectively, for niobium; and 183.84 g/mol and 19.35 g/cm^3, respectively, for tungsten.

Question V: Microstructural Characterization

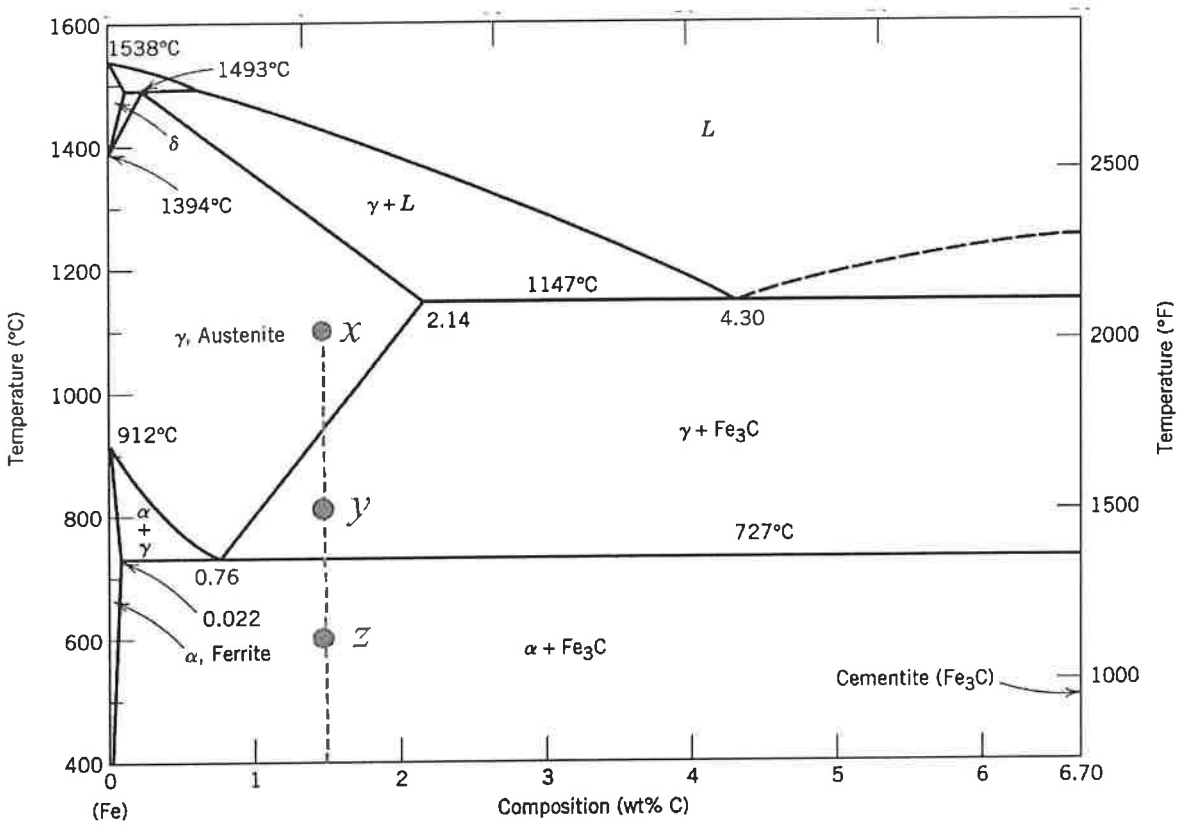
1. (**12 marks**) The X-ray diffraction for an element that has either the BCC or the FCC crystal structure shows diffraction peaks at the following 2θ angles: 40, 58, 73, 86.8, 100.4, and 114.7. The wavelength of the incoming ray was 0.154 nm.
   a. (**6 marks**) Determine the cubic structure of the element.
   b. (**6 marks**) Determine the lattice constant of the element.
2. (**2*4 = 8 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, and (c) resolution and magnification. (d) Which of these can reveal details on sub-surface dislocation activity in a metallic thin sample?

Question VI: Dislocations and Grain Boundaries

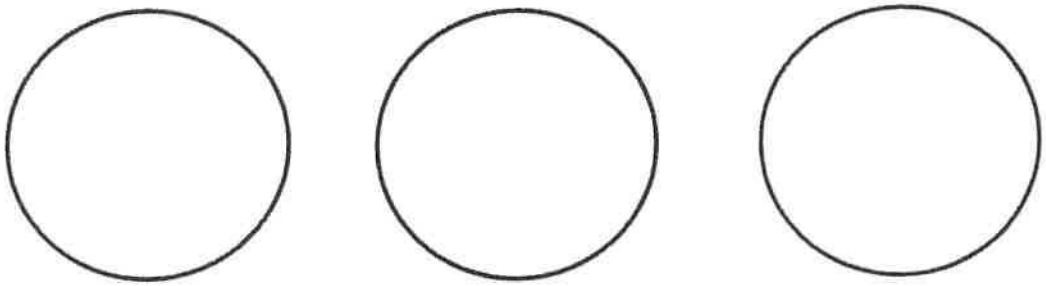
1. (**8 marks**) This question pertains to dislocations
   a. (**4 marks**) Differentiate between screw and edge dislocations. Which one is expected to dominate during torsional deformation of an FCC solid?
   b. (**4 marks**) What is meant by Burger's vector? Write down Burger's vectors for screw and edge dislocations in Cu, in terms of its lattice constant, a.
2. (**12 marks**) This question pertains to the deformation mechanisms of crystalline solids.
   a. (**2 marks**) Define deformation by twinning.
   b. (**6 marks**) Indicate the slip systems that are responsible for deformation in pure Cu (FCC). Support your answer with an illustration of the appropriate planes with slip directions clearly labelled schematically.
   c. (**4 marks**) A brass alloy consisting of 70%Cu-30%Zn with an average grain size 100 μm has a yield strength of 64.5 MPa. If through some processing, the average grain size of a material is reduced to 50 nm, what will be the yield strength of the new microstructure? $\sigma_0 = 25$ MPa.

Question VII: Phase Diagram

(**20 marks**) For the binary phase diagram for iron-carbon shown below, answer the following questions:



1. (**5 marks**) Where are the invariant points on this phase diagram? (indicate temperature and composition). Write down the eutectic and eutectoid reactions. Indicate temperature and %C concentrations where these reactions occur.
2. (**5 marks**) For a sample of 1.5 wt% C steel at 1100°C (point x), what phase(s) will be present, and what will be the composition of each phase, in wt% C?
3. (**5 marks**) If this alloy is cooled from 1100°C along the dotted line, as shown in above figure, schematically draw the microstructure at points *x*, *y*, and *z*, as if you are filling following circles. Identify phases in each microstructure.



At point *x* At point *y* At point *z*

4. (**5 marks**) For the microstructure formed at point z, what is the fraction of pearlite and proeutectoid cementite?

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

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

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

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

$N_D = N\exp\left(-\dfrac{Q_D}{kT}\right)$ $N = \dfrac{\rho N_A}{A_{wt}}$; 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