Engineering 45: Properties of Materials
Final Exam
May 9, 2012

Name:

Student ID number:

Instructions: Answer all questions and show your work. You will not receive partial credit unless you show your work. Good luck!

1a (4 points)	
1b (4 points)	
1c (8 points)	
1d (8 points)	
2a (4 points)	
2b (4 points)	
2c (4 points)	
2d (4 points)	
2e (6 points)	
3a (6 points)	
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3c (6 points)	
3d (4 points)	
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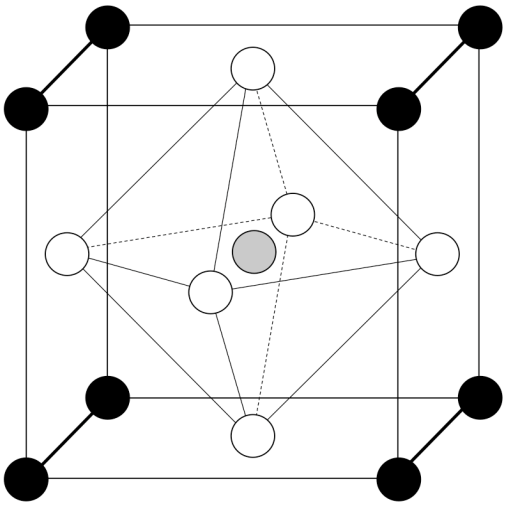
4a (4 points)	
4b (4 points)	
4c (4 points)	
4d (4 points)	
4e (4 points)	
4f (4 points)	
4g (4 points)	
Total (100 points)	

Problem 1: $NaTaO_3$ is a compound with the cubic perovskite crystal structure shown in the figure below. Use the information given to answer parts (a) – (e) on pages 2-5.

(a) (4 points) Assuming that the bonding is ionic, give the charge and electron configuration for each ion (Na, Ta and O).



Cubic perovskite structure of $NaTaO_3$. Black circles denote Na ions at cube corners, the grey circle denotes the Ta ion at the body center, and the white circles denote O ions at face centers.

Problem 1 (continued)

(b) (4 points) Determine the maximum radius of an impurity atom that can fit in the interstitial site at ¼ ¼ ¼. Assume that the lattice constant is 4.00 Å and the ionic radii are as follows: Na (1.4 Å), Ta (0.6 Å), O (1.4 Å). Give your answer in Å units.

Problem 1 (continued)

(c) (8 points) The addition of Bi^{3+} impurities to $NaTaO_3$ leads to an increase in the diffusion constant for oxygen ions. It is known that oxygen ion diffusion occurs by a vacancy mechanism.

i. Determine if Bi^{3+} substitutes for Na or Ta in the lattice, and explain your answer.

ii. Give an expression for the diffusion constant in terms of the attempt frequency (ν), the mole fraction of Bi impurities [Bi^{3+}] the lattice constant (a), the migration energy (Q_m), Boltzmann's constant (k) and temperature (T). Assume all oxygen vacancies come from the added impurities.

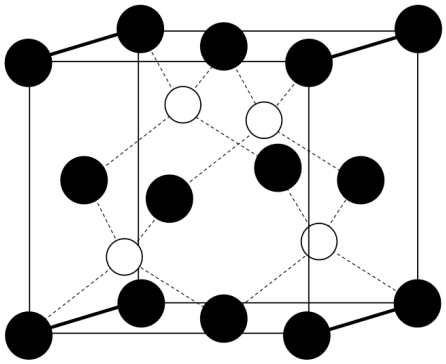
Problem 1 (continued)

(d) (8 points) For wavelengths of light (λ) below 320 nm the absorbance A (fraction of light absorbed) in a carefully synthesized single crystal of $NaTaO_3$ is 0.8, while for $\lambda > 320$ nm A=0. Using this information, compute (i) the dielectric constant (ε_r) and (ii) the band gap (E_{gap}) of this material.

Problem 2: ZnTe is a compound semiconductor that forms in the cubic zincblende crystal structure shown below. The material is red in color and has a band-gap of E_{gap} = 2.2 eV. Use the information provided to answer parts (a) – (e) on pages 6-8.

(a) (4 points) Sketch the atomic configuration for a {110} plane in the zincblende structure and determine the number of broken nearest-neighbor bonds per unit area at a {110} surface.

(b) (4 points) Which of following impurities would you expect to be donors and which would you expect to be acceptors in ZnTe: P, Al, Cu? Indicate for which atom (Zr or Te) the dopants are likely to substitute.



Zincblende structure of ZnTe. Zn and Te are denoted by black and white spheres, respectively.

Problem 2 (continued)

(c) (4 points) Consider a ZnTe compound doped with P impurities. Sketch the energy levels for this doped compound in the space provided below. Label the valence band, the conduction band, the bandgap and the positions of the P impurity levels.

(d) (4 points) On the space provided below, sketch the carrier concentration versus temperature for the compound in part (c). On your sketch label the freeze-out, extrinsic and intrintsic regimes, and give the numerical value of the carrier concentration in the extrinsic regime (in units of m^{-3}). The P dopant concentration is 1.5×10^{24} m^{-3}.

Problem 2 (continued)

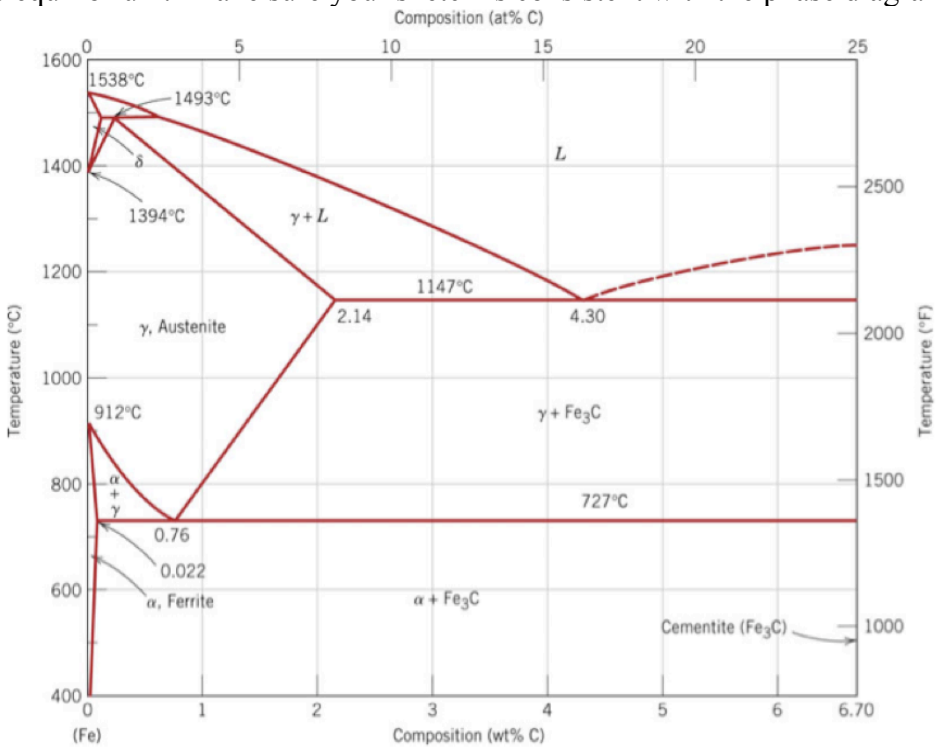
(e) (6 points) For the doped compound considered in parts (c) and (d), the resistivity at a temperature of 400°C, which is within the extrinsic regime, is 8.3×10^{-4} Ω·m.

i. (4 points) Compute the resistivity at 400°C for undoped (intrinsic) ZnTe assuming that the mobilities of holes and electrons are equal. At 400°C the lattice constant of ZnTe is 6.10 Å. Assume that the intrinsic carrier concentration is given as $n_i = p_i = N \exp(-E_{gap} / 2kT)$, where N is the atomic density.

ii. (2 points) Will the intrinsic conductivity increase or decrease with increasing temperature? Explain.

Problem 3: In this problem you will consider microstructure and phase equilibria in Fe-C. Answer parts (a)-(e) on pages 9-13.

(a) (6 points) Shown below is the phase diagram for Fe-C. In the space provided, plot free-energy curves for ferrite, austenite and cementite phases at a temperature of 800°C. On your sketch show relevant common tangents and label the regions of single and two-phase equilibrium. Make sure your sketch is consistent with the phase diagram.

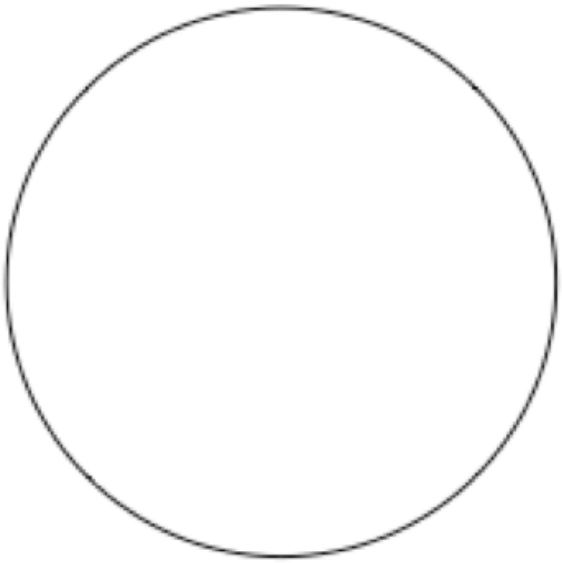


Problem 3 (continued)

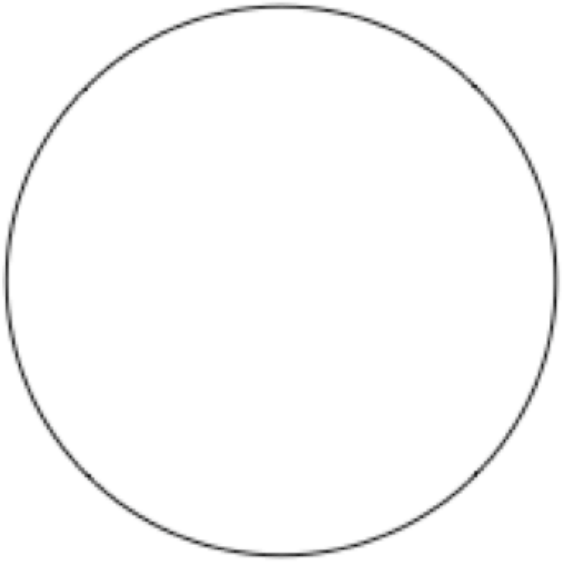
(b) (6 points) Consider an alloy with 1.5 wt. % C, that is cooled slowly from the melt. List the phases present, their composition, and the weight fraction of each phase at the following four temperatures: 1600^{o}C, 1100^{o}C, 800^{o}C and 400^{o}C.

Problem 3 (continued)

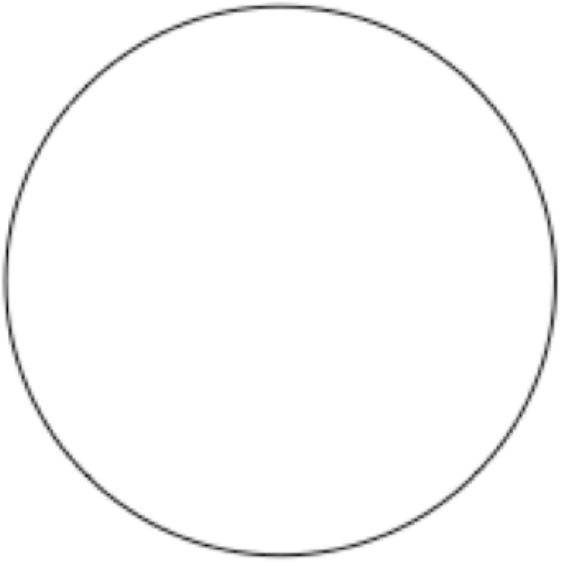
(c) (6 points) For the alloy considered in part (b) sketch the microstructures in the space provided at 1100°C, 800°C and 400°C. Be sure to label each phase present. Your sketches should be qualitatively consistent with your results for part (b). Show grain boundaries on your sketches where you expect polycrystalline microstructures.



T=1100°C



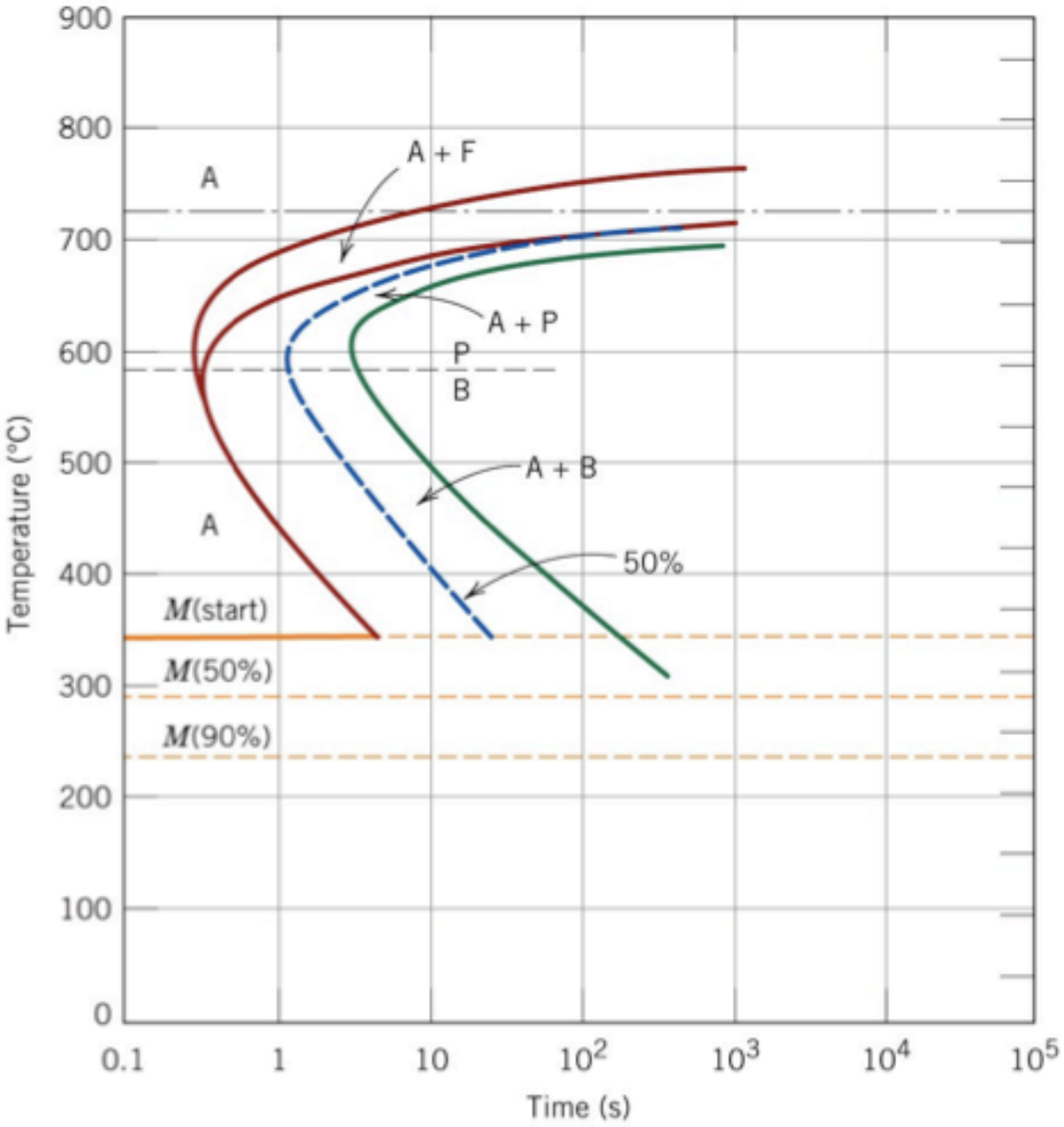
T=800°C



T=400°C

Problem 3 (continued)

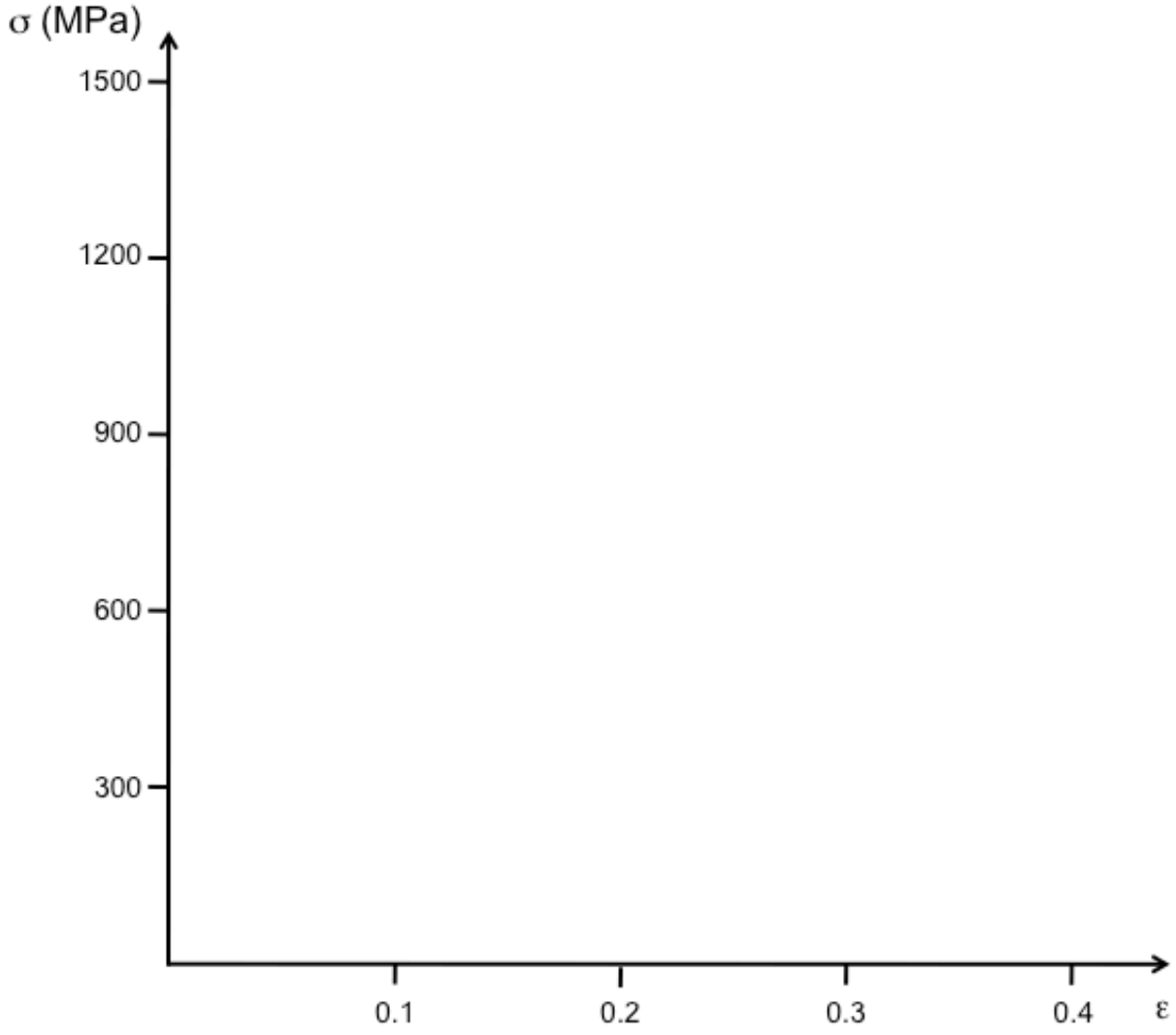
(d) (4 points) Shown below is a TTT diagram for a hypoeutectoid Fe-C alloy. On the diagram draw a time-temperature path that could be used to produce (i) a tempered martensite microstructure, (ii) a microstructure with 50 % proeutectoid ferrite and 50 % coarse pearlite, and (iii) a spheroidite microstructure with minimal proeutectoid ferrite.



(e) (4 points) It is observed experimentally that the hardness of a steel with a spheroidite microstructure decreases with the amount of aging time. Using your knowledge of hardening mechanisms explain why this might be. Assume there is negligible grain growth during aging and that the steel has not been cold worked.

Problem 4: Consider a Co-Cr alloy used for vascular stent applications. The alloy has a plane-strain facture toughness of K_{Ic} = 60 MPa·√m, a yield strength of σ_{yield} = 547 MPa, an ultimate tensile strength of 1449 MPa, a Young's modulus of E = 243 GPa, a 30% total elongation at failure, and a fatigue limit of S_{fat} = 200 MPa. Use the information provided to answer parts (a) – (e) on pages 14-17.

(a) (4 points) In the space provided below sketch a tensile stress-strain curve for this alloy. Label the values of the yield strength, the ultimate tensile strength, and the plastic strain at failure. Also label the regions of (I) elastic, (II) stable plastic and (III) unstable plastic deformation.



Problem 4 (continued)

(b) (4 points) What features of the tensile stress-strain curve shown in your answer to part (a) would change if the alloy was cold worked? Explain your answer.

Problem 4 (continued)

(c) (4 points) When the stent is inserted into a blood vessel, an expandable balloon is used to impose a stress on the stent that will expand it to near final shape. What is the minimum tensile stress that the balloon needs to impose on the material for reshaping? What is the maximum tensile stress it can impose without breaking the stent?

(d) (4 points) It is critical that the stress imposed in the shaping procedure does not lead to fracture of the stent. If the maximum tensile stress imposed during this process if 1400 MPa, estimate the critical length of a pre-existing crack that would lead to fracture.

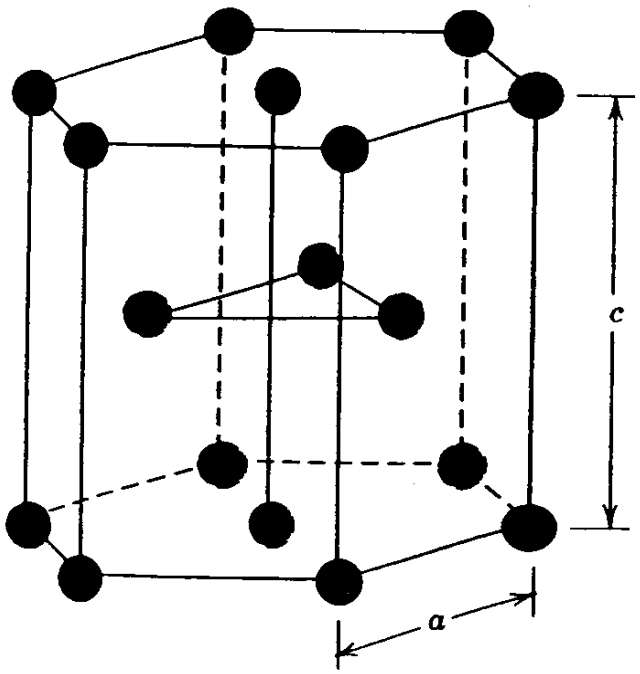
Problem 4 (continued)

(e) (4 points) After insertion the stent experiences cyclic loading tied to the heartbeat, with a stress amplitude of S=52 MPa under normal blood-flow conditions. Do you expect that fatigue failure is a concern if the stent is intended to survive for 10 years given an average heart rate of 70 beats per minute? Explain your answer using a sketch of the *S*-*N* plot for this alloy.

(f) (4 points) Calculate the critical resolved shear stress (τ_{CRSS}) for this alloy assuming that the yield strength corresponds to the applied stress when yielding begins in the most favorably oriented grains in the polycrystalline microstructure.

Problem 4 (continued)

(g) (4 points) The Co-Cr alloy has an hcp crystal structure. On the figure of the hcp structure below draw six possible slip directions and label the most favorable type of slip plane. Explain your answers.



Formulas, Constants, and Definitions

Constants and Units

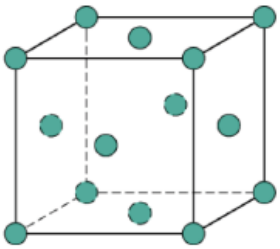
- *Boltzmann Constant*: $k = 1.3806 \times 10^{-23}$ J / K = 8.6173×10^{-5} eV / K
- *Avogadro's Number*: $N_A = 6.022 \times 10^{23}$ atoms / mol
- *Atomic Mass*: 1 amu = 1 g / mol
- *Planck's Constant*: $h = 4.136 \times 10^{-15}$ eV s
- *Speed of Light*: $c = 2.998 \times 10^{8}$ m / s
- *Electron charge*: $|e| = 1.602 \times 10^{-19}$ C
- 1 Ω = 1 J · s / C^2

Bonding

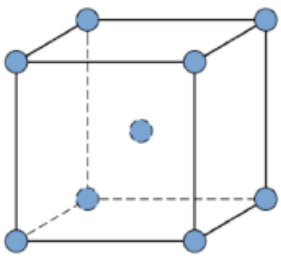
- *Types of Primary Bonding*: Ionic, Covalent, Metallic
- *Secondary Bonding*: Dipole-Dipole, Hydrogen, Dipole-Induced Dipole, Fluctuating Dipole

Crystallography

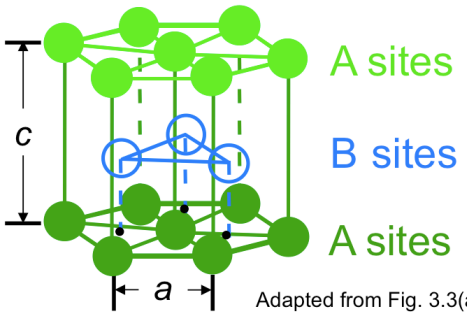
- *Bragg's Law*: $2\, d_{hkl} \sin\theta = n\, \lambda$
- *Interplanar Spacing in Cubic Crystals*: $d_{hkl} = a / (h^2 + k^2 + l^2)^{1/2}$
- *FCC Structure* (ABCABCABC…):



- *BCC Structure*:



- *HCP Structure* (ABABAB…):



Adapted from Fig. 3.3(a), *Callister & Rethwisch 3e.*

- *Point Coordinates*: ijk
- *Crystallographic Directions*: [ijk]
- *Family of Crystallographic Directions*: <ijk>
- *Miller Indices for Planes*: (hkl)
- *Family of Planes*: {hkl}

Defects

- *Point Defects*: Vacancies, Impurities, Interstitials, Shottky Defect, Frenkel Defect
- *Line Defects*: Screw Dislocation (*b* parallel to *L*), Edge Dislocation (*b* perpendicular to *L*), Mixed Dislocation (*b* at angle to *L* other than zero or 90 degrees)
- *Planar Defects*: Surfaces, Grain Boundaries, Stacking Faults, Twins, Two-Phase Interfaces
- *Equilibrium Vacancy Concentration*: $c_v^e = N_v^e / N = \exp[\ Q_v / kT]$
- *Equilibrium Concentration of Schottky Defects in a Metal Oxide*: $N_s = N \exp(-Q_s / 2kT)$

Phase Diagrams

- *Lever Rule*: $W_\alpha = \dfrac{C_0 - C_\beta}{C_\alpha - C_\beta}; \quad W_\beta = \dfrac{C_\alpha - C_0}{C_\alpha - C_\beta}$

Kinetics

- *Temperature Dependence of Diffusion Constant*: $D = D_0 \exp[-Q_d / kT]$
- *Relation Between Diffusion Constant, Jump Rate (ω) and Jump Distance (r)*: $D = \dfrac{1}{6} r^2 \omega$
- *Jump Rate for Interstitial Diffusion*: $\omega = v \exp[-Q_m / kT]$
- *Jump Rate for Substitutional-Impurity Diffusion and Self-Diffusion by vacancy mechanism*: $\omega = v[c_V] \exp[-Q_m / kT]$

Electronic Properties

- *Conductivity:* $\sigma = n\ |e|\ \mu_e + p\ |e|\ \mu_h$, where n and p are electron and hole carrier concentrations, and μ_e and μ_h are electron and hole mobilities.

- *Intrinsic Carrier Concentrations*: $n_i = p_i = N \exp(-E_{gap} / 2kT)$, where N is the atomic density.

Optical Properties

- *Conservation of Energy in terms of intensities of incident, reflected, absorbed, scattered and transmitted light intensities*: $I_0 = I_R + I_A + I_S + I_T$

- *Relationship Between Speed of Light, Wavelength (λ) and Frequency (ν)*: $c = \lambda \nu$

- *Energy of Photon*: $E = h \nu$

- *Relationship Between Index of Refraction (n) and Dielectric Constant (ε_r)*: $n^2 = \varepsilon_r$

- *Snell's Law*: $n_1 \sin(\theta_1) = n_2 \sin(\theta_2)$

- *Reflectance (Fraction of Incident Light Reflected)*: $R = [(n\text{-}1)/(n\text{+}1)]^2$

Mechanical Properties

- *Young's Modulus (E) in Linear Elastic Regime*: $\sigma = E\ \varepsilon$

- *Relationship Between Shear Strain (γ), Shear Stress (τ) and Shear Modulus (G)*: $\tau = G\ \gamma$

- *Yield Stress (σ_{yield})*: Stress at which plastic strain is $\varepsilon_P = 0.002$

- *Resolved Shear Stress*: $\tau_R = \sigma \cos(\lambda) \cos(\phi)$ where λ is angle from tensile axis to slip direction and ϕ is angle between tensile axis and normal to slip plane

- *Hall-Petch Equation*: $\sigma_{yield} = \sigma_0 + k_y d^{-1/2}$ where d is the grain size

- *Solid Solution Strengthening*: increase in $\sigma_{yield} \sim C^{1/2}$ where C is solute concentration

- *Precipitation Hardening*: increase in $\sigma_{yield} \sim 1 / S$ where S is distance between precipitates

- *Strain Hardening*: σ_{yield} increases with increasing dislocation density

- *Griffith Criterion*: $\sigma_c = (2E\gamma_s / \pi a)^{1/2}$ where E is Young's modulus, γ_s is the surface energy, and a is crack length.

- *Fracture Criterion Based on Plain-Strain Fracture Toughness*: $\sigma_c = K_{IC} / [Y (\pi a)^{1/2}]$ where K_{IC} is the fracture toughness, a is crack length, and Y is a shape factor that can be taken as one.

IA																	0
1 H 2.1	IIA							VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	2 He –
3 Li 1.0	4 Be 1.5												5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne –
11 Na 0.9	12 Mg 1.2	IIIB	IVB	VB	VIB	VIIB							13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar –
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.8	28 Ni 1.8	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr –
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5	54 Xe –
55 Cs 0.7	56 Ba 0.9	57–71 La–Lu 1.1–1.2	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.8	83 Bi 1.9	84 Po 2.0	85 At 2.2	86 Rn –
87 Fr 0.7	88 Ra 0.9	89–102 Ac–No 1.1–1.7															

Periodic Table of the Elements with electronegativity values included. Reproduced from Callister.

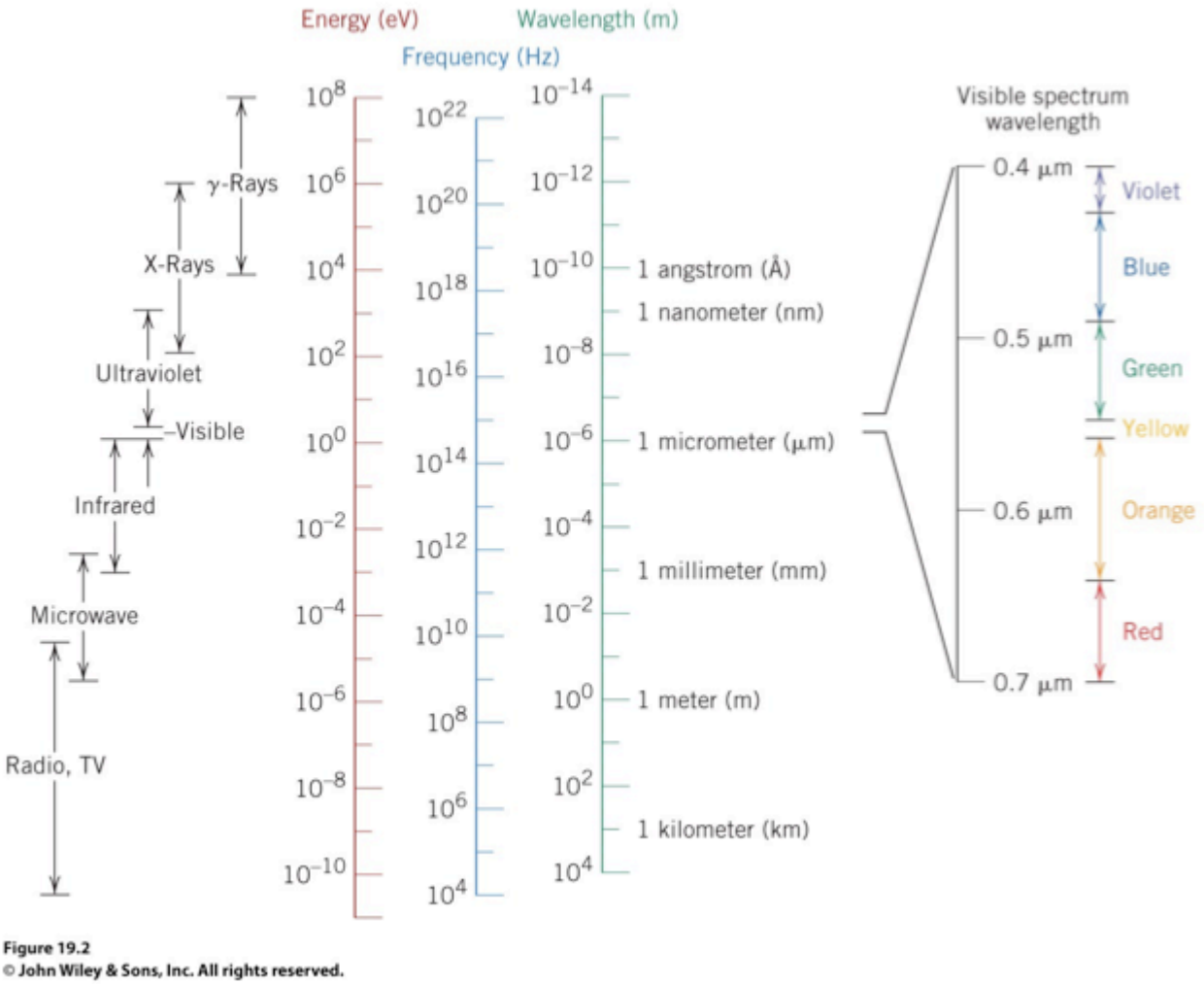


Figure 19.2

Electromagnetic Spectrum. Reproduced from Callister.