

Matsci 45: Properties of Materials
Final Exam
May 8, 2024

Name:

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SID:

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Instructions:

- Answer all questions and show your work to receive full credit.
- Write your answers in the boxes provided.
- Good luck!

Problem & Points	Score	Problem & Points	Score
1a: 5 points		2g: 2 points	
1b: 2 points		2h: 2 points	
1c: 3 points		2i: 3 points	
1d: 4 points		3a: 4 points	
1e: 4 points		3b: 6 points	
1f: 3 points		3c: 2 points	
1g: 5 points		3d: 3 points	
1h: 4 points		4a: 3 points	
2a: 4 points		4b: 6 points	
2b: 2 points		4c: 7 points	
2c: 6 points		4d: 5 points	
2d: 4 points		Total: 100 points	
2e: 4 points		5 (extra credit): 10 points	
2f: 7 points			

1. This problem concerns the material CaF_2 , which forms in the cubic fluorite crystal structure shown in Figure 1. Ca is arranged in an fcc crystal structure and all of the tetrahedral interstitial sites are occupied by F. The arrows in Figure 1 indicate crystallographic directions $x=[100]$, $y=[010]$ and $z=[001]$. The lattice constant ($a=0.561$ nm) and ionic radii for Ca and F are given below (note that the sizes of Ca and F spheres are not drawn to scale).

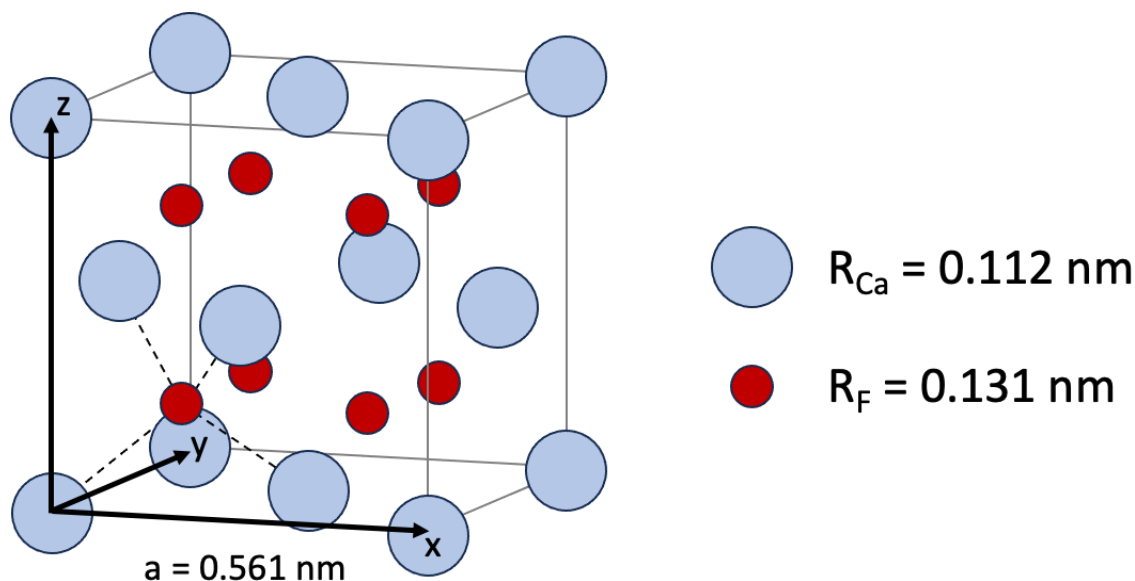


Figure 1: Cubic fluorite crystal structure of CaF_2 . The dashed lines illustrate tetrahedral coordination for one of the F ions (note that all F ions have the same coordination).

- a. Determine the number of Ca and F ions in the unit cell, and compute the atomic packing fraction. List your answers in the boxes and show your work in the space provided.

Number of Ca:

Number of F:

Atomic packing fraction (give 3 significant figures):

Space for work

Problem 1 Continues on the next page



- b. On Figure 1, label with a number (1) the ion at position $\frac{1}{4} \frac{1}{4} \frac{1}{4}$, and with a number (2) the ion at position $0\frac{1}{2}\frac{1}{2}$.
- c. In the box below list the direction (using proper notation) in the crystal that connects the ion at the origin to the ion at position $\frac{3}{4}\frac{1}{4}\frac{1}{4}$.

List the direction

- d. In the space provided below, draw the atomic pattern on the (020) plane. Label the ion types, and indicate with an X symbol the position of the octahedral interstitial site at the crystallographic position $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.



- e. Assuming ionic bonding what is charge on Ca and F and what are the electron configurations on these ions?

Ca Ion Charge:

F Ion Charge:

Ca Ion e⁻ Config:

F Ion e⁻ Config:

Problem 1 Continues on the next page



- f. The dominant (highest concentration) intrinsic point defect in CaF_2 is an anion Frenkel, composed of a F vacancy and a F interstitial. Which of the following are likely factors contributing to this defect having the highest concentration compared to other possible point defects:

- (i) The formation energy of the anion Frenkel is higher than that for other possible point defects.

List True (T) or False (F)

- (ii) The octahedral interstitial site is large enough for F ions to fit in it.

List True (T) or False (F)

- (iii) The octahedral interstitial site is surrounded by nearest-neighbor cations, favoring ionic bonding with an anion interstitial.

List True (T) or False (F)



Figure 2: Optical lenses made of CaF_2 . The optical properties of CaF_2 are considered in Problem 1g. Image from <https://global.canon/en/c-museum/special/exhibition2.html>.

Problem 1 Continues on the next page



g. CaF_2 finds application as a material for high performance lenses (see Fig. 2) in cameras and telescopes. Two properties that make it attractive for this application are: (1) it does not absorb light for any of the visible wavelengths, and (2) it has a small dielectric constant of $\epsilon_r = 1.4$ that does not vary strongly with wavelength, leading to small reflectance and low refraction of light across visible wavelengths.

- (i) Given this information, what is the smallest possible value of the bandgap of CaF_2 ? List your answer in the box, and explain your answer briefly in the space provided. Note: the energy spectrum for visible light is given in Table 1 on the next page.

Minimum value of bandgap in eV units (to 2 sig figs)

Brief explanation for answer:

- (ii) Given the information above, compute the reflectance R .

Value of R (to 3 sig figs)

Space for your work:

Problem 1 Continues on the next page



Table 1: Wavelengths and energy of visible light (from K.Nassau, “Experimenting with Color”)

COLOR	WAVELENGTH	ENERGY
Red	700 nm	1.771 eV
Reddish orange	650 nm	1.909 eV
Orange	600 nm	2.067 eV
Yellow	580 nm	2.138 eV
Yellowish green	550 nm	2.254 eV
Green	500 nm	2.480 eV
Blue	450 nm	2.765 eV
Violet	400 nm	3.100 eV

Problem 1 Continues on the next page



- h. One of the challenges with the use of CaF_2 lenses is that they are fragile and can break (fracture) under stress. Engineering reports have documented a fracture strength of $\sigma_c = 34.1$ MPa for coarse polished versus $\sigma_c = 157.2$ MPa for well polished samples. Using the appropriate failure criterion for a brittle ceramic, determine the maximum surface flaw size (a) for (i) coarse polished and (ii) well polished samples. For CaF_2 the elastic modulus is $E = 75.8$ GPa and the surface energy is $\gamma_s = 0.750$ J/m². Note: 1 GPa = 10^9 Pa, 1 MPa = 10^6 Pa, and 1 Pa = 1 J/m³.

Flaw size for coarse polished (in m, to 3 sig figs):

Flaw size for well polished (in m, to 3 sig figs)

Space for work

2. Shown in Figure 3 is the Fe-C phase diagram for compositions between Fe and Fe₃C.

a. The diagram features one eutectic reaction, and one eutectoid equilibrium:

i. Eutectic: $L \rightleftharpoons \gamma + \text{Fe}_3\text{C}$

ii. Eutectoid: $\gamma \rightleftharpoons \alpha + \text{Fe}_3\text{C}$

For each of these two invariant equilibria (i) and (ii), give the temperature (in °C), and the compositions (in wt.% C) of each phase involved:

Eutectic

Temperature	Composition (L)	Composition (γ)	Composition (Fe ₃ C)

Eutectoid

Temperature	Composition (γ)	Composition (α)	Composition (Fe ₃ C)

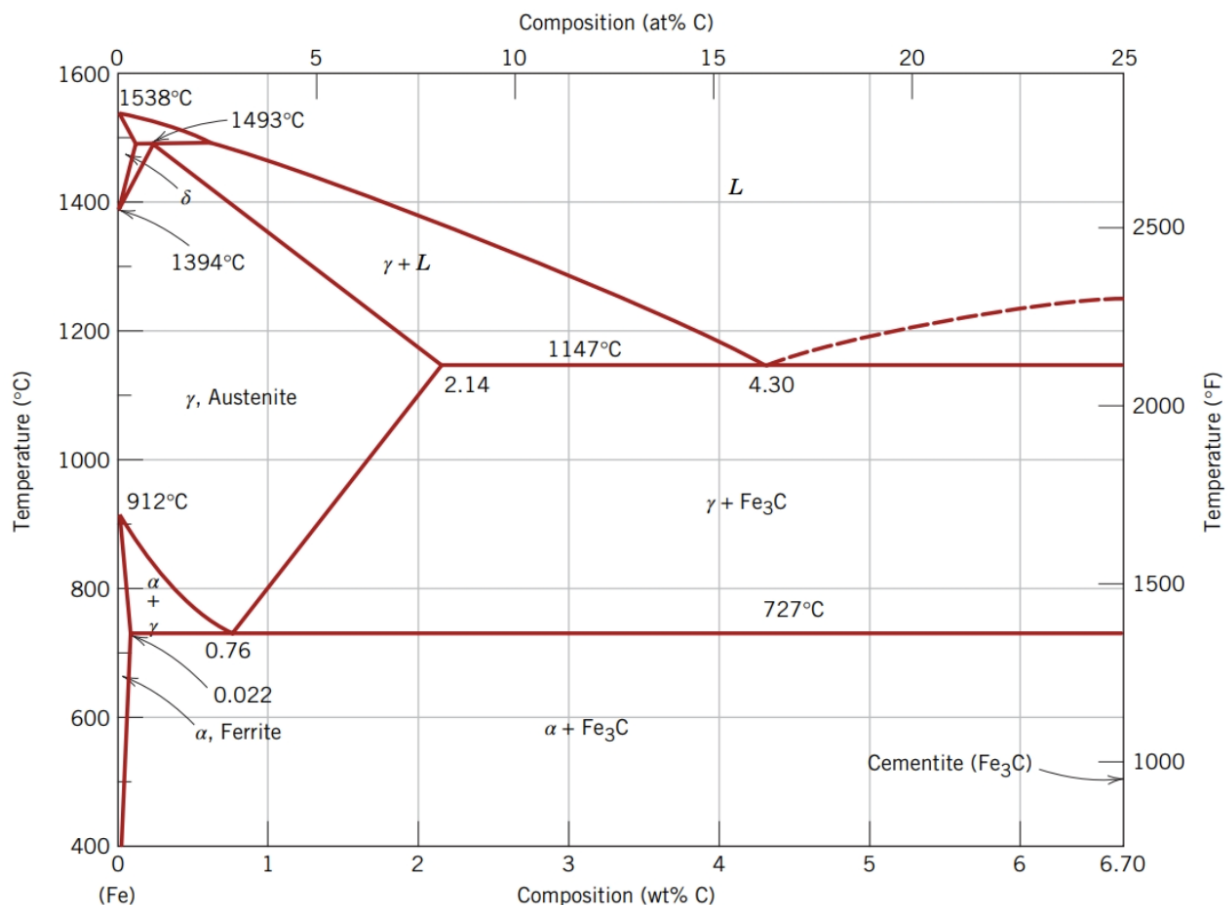


Figure 3: Fe-C phase diagram, reproduced from Callister

Problem 2 Continues on the next page



- b. Figure 4 below shows a microscopy image of the microstructure resulting from slow cooling from the austenite (γ) phase, for a hypereutectoid Fe-C alloy. In this image, the lighter regions are Fe_3C phases and the darker are ferrite (α). In the boxes in Figure 4 list which microconstituent corresponds to proeutectoid Fe_3C and which corresponds to pearlite.

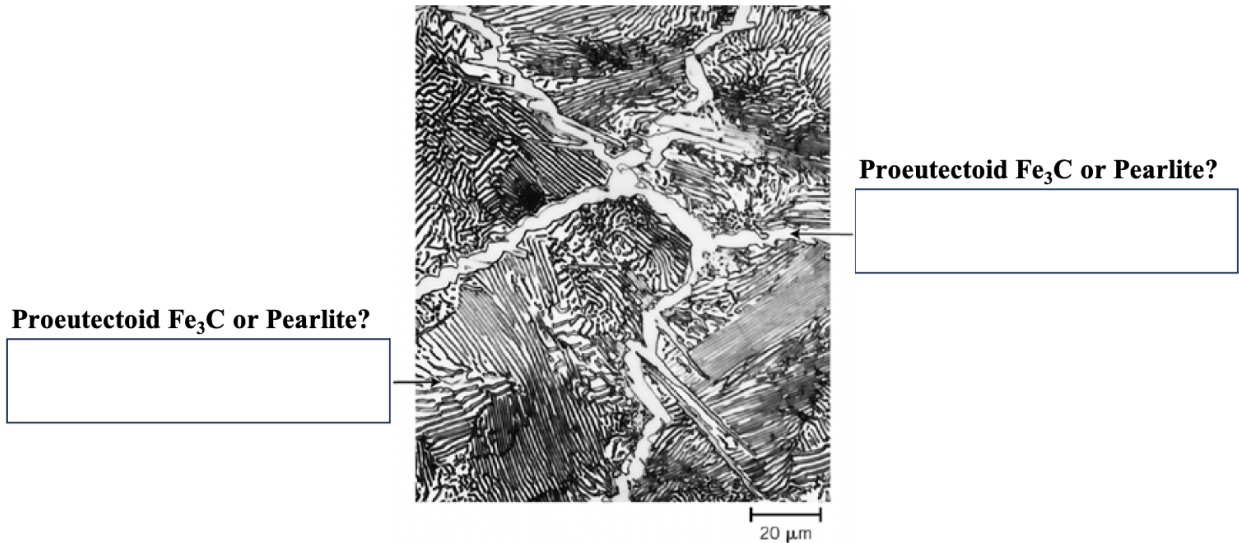


Figure 4: Microscopy image of a hypereutectic Fe-C alloy resulting from a slow cool from the austenite (γ) phase. The light regions are Fe_3C and the dark regions are ferrite (α).

Problem 2 Continues on the next page



- c. The alloy in Figure 4 has composition 1.40 wt.% C.
- i. In the space provided, compute the weight fractions of the ferrite (α) phase and the weight fraction of the cementite Fe_3C phase at the eutectoid temperature for this alloy.

Weight fraction α (to 3 sig figs)

Weight fraction Fe_3C (to 3 sig figs)

Space for work

- ii. Compute also the weight fraction of the pearlite microconstituent in the microstructure.

Weight fraction pearlite (to 3 sig figs)

Space for work

Problem 2 Continues on the next page



- d. Shown in Fig. 5 is the tensile stress-strain curve for an alloy with composition 0.38wt.% C, featuring a yield strength of $\sigma_{\text{yield}} = 250$ MPa, an ultimate tensile strength of TS = 450 MPa, and a ductility corresponding to 37% elongation. On Figure 5, sketch a tensile stress-strain curve for the alloy with a composition of 1.40wt.% C, assuming the following: (i) it has the same Young's modulus as the alloy with composition 0.38wt.% C, (ii) $\sigma_{\text{yield}} = 350$ MPa, (iii) TS = 500 MPa and (iv) the ductility corresponds to 30% elongation.

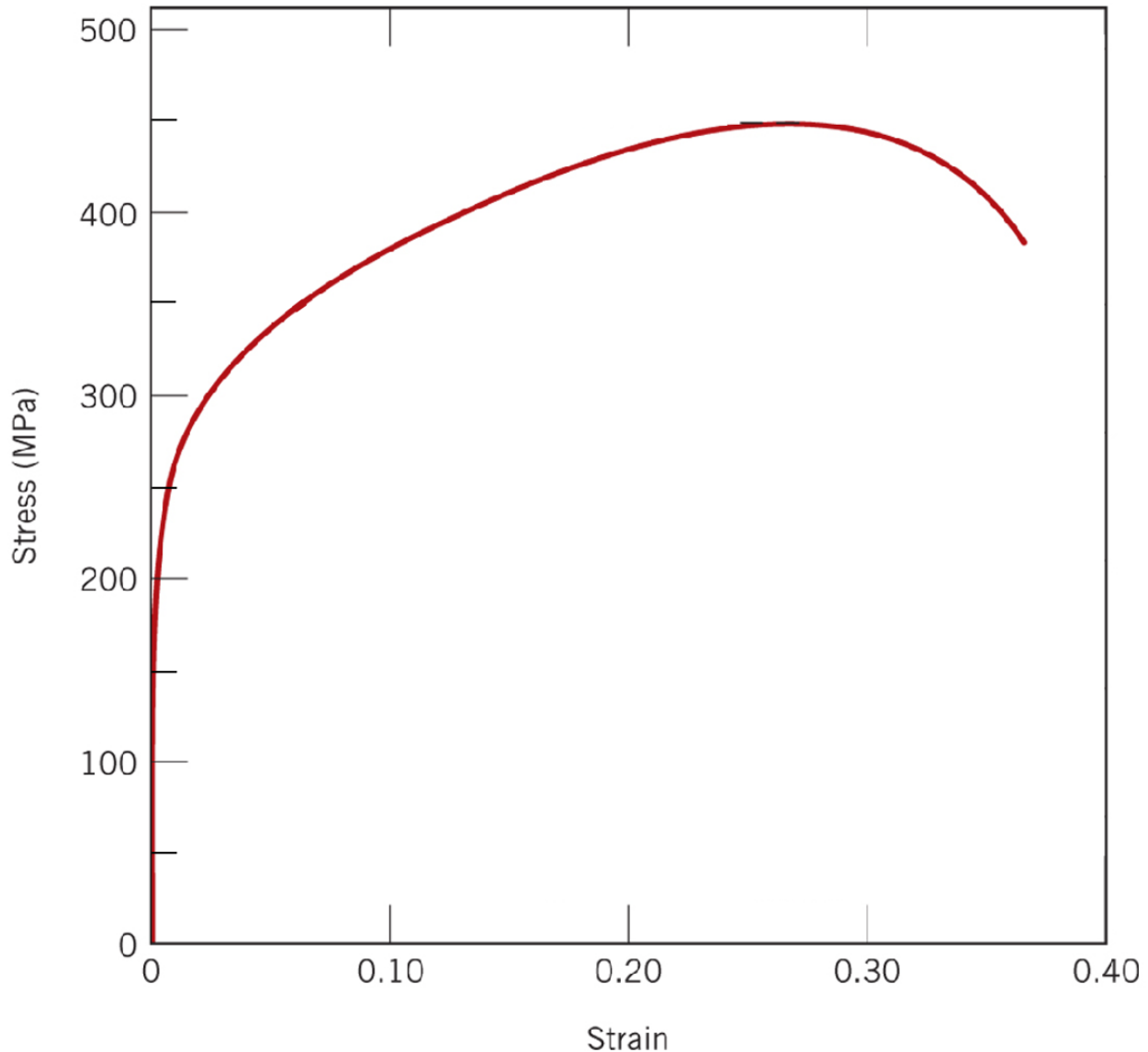


Figure 5: Tensile stress-strain curve plotting engineering stress (y-axis) versus engineering strain (x-axis). For use in problem 2.d.

Problem 2 Continues on the next page



- e. We will consider again the alloy with composition 0.38wt.% C, featuring the mechanical properties given in part (d). Suppose also that the fracture toughness for this alloy has a fracture toughness value of $K_{IC} = 50 \text{ MPa m}^{1/2}$ (where $1 \text{ MPa} = 10^6 \text{ Pa}$).
- i. If we have a rod of the material with cross-sectional area $A = 1 \text{ m}^2$ (see Figure 6) what is the maximum load (F) that can be applied before we reach the value of the ultimate tensile strength (TS). (Recall that $1 \text{ Pa} = 1 \text{ N} / \text{m}^2$).

Maximum load (in N to 3 sig figs)

Space for calculation:

- ii. Suppose we have a crack of size $2a = 1 \text{ mm}$ inside the rod. Compute the fracture stress (assuming shape factor of one).

Fracture stress (in MPa units, to 3 sig figs)

Space for calculation:

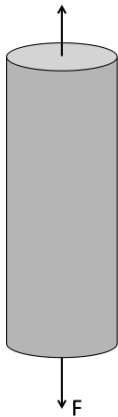


Figure 6: schematic for problem 2.e.

Problem 2 Continues on the next page



- f. Suppose now that we want to increase the surface hardness of the alloy with $C_0=0.38\text{wt.\% C}$, through carburization. This process involves exposing the surface to a carbon rich gas, leading to a fixed value of the surface concentration, C_s (where $C_s > C_0$), and diffusion of carbon into the material. Figure 7 plots the concentration profile after carburizing for a time $t_1 = 10$ minutes at a temperature of $T = 700^\circ\text{C}$. The distance $x_1 = (Dt_1)^{1/2}$ is identified where the carbon concentration takes a value of $(C_0 + C_s)/2$.
- i. Compute the value of x_1 if we have the following values for the prefactor and activation energy for C diffusion in the alloy: $D_0 = 1.10 \times 10^{-6} \text{ m}^2/\text{s}$, $Q_d = 0.906 \text{ eV}$. Recall the value of the Boltzmann Constant: $k = 8.6173 \times 10^{-5} \text{ eV / K}$, and you can convert from $^\circ\text{C}$ to K units of temperature by adding 273K.

Value of x_1 (in m, to 3 sig figs)

Space for work

- ii. Sketch on Figure 7 the composition profile at time $t_2 = 4t_1$. On your sketch note the value of x where the concentration takes a value of $(C_0 + C_s)/2$ at time t_2 .

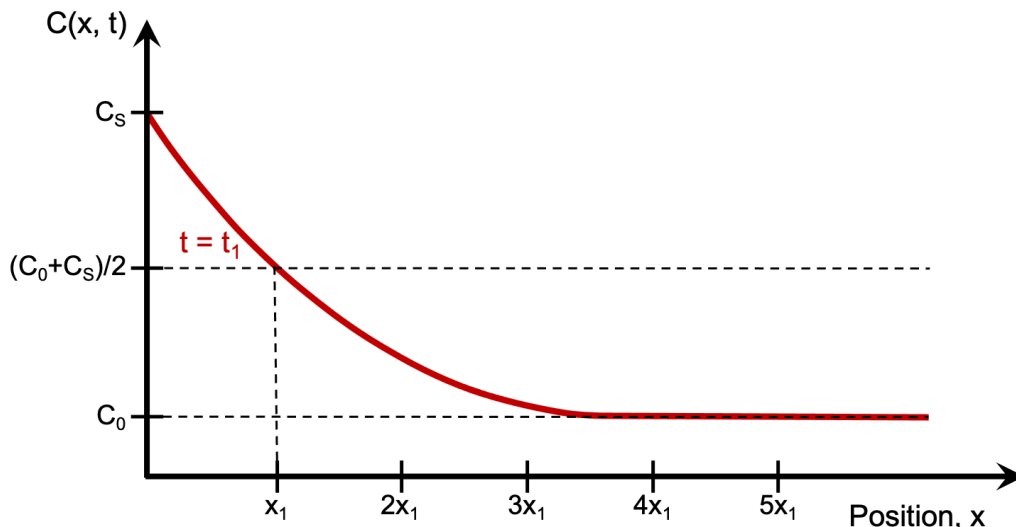


Figure 7: Carbon concentration resulting from carburizing at 700°C .

Problem 2 Continues on the next page



- g. Suppose that the process of carburization has two effects, namely increasing the carbon concentration in the α phase, and causing the formation of small particles of second-phase carbide in α . All other microstructural features stay the same. In this case which of the following are the main strengthening mechanisms associated with carburization (there is only one correct answer):

- i. Solid-solution strengthening
- ii. Precipitation strengthening
- iii. Both (i) and (ii)
- iv. Grain boundary strengthening
- v. Work hardening
- vi. All of the above

Answer (i, ii, iii, iv, v, or vi; there is only one correct answer):

- h. Before carburization the steel has a fatigue lifetime plot like that shown in Figure 8. On this figure, sketch a curve illustrating how this curve might look after carburization.

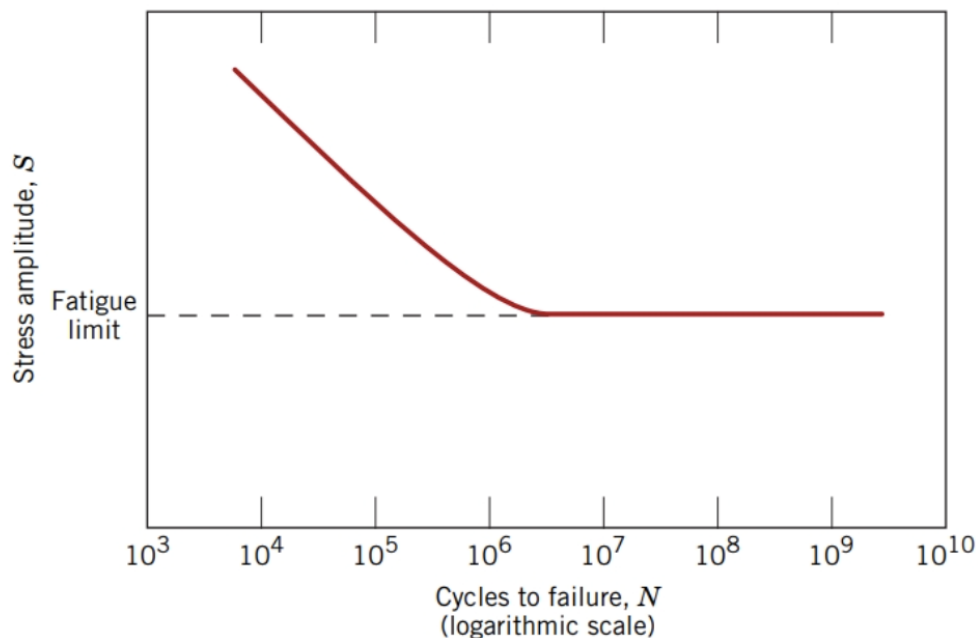


Figure 8: Dependence of fatigue lifetime on stress amplitude during cyclic loading for the Fe-C considered in problem 2 e-g.

Problem 2 Continues on the next page



- i. The α phase of Fe-C has a body-centered-cubic (bcc) structure. The (110) plane is the most close-packed plane in the bcc structure. Carbon atoms have a size that is much smaller than that of iron atoms, and carbon fits into the octahedral interstitial sites. Given all of this information, which of the following are true statements?

- (i) The Burgers vector (**b**) for dislocations in this structure is **b** = $a \langle \frac{1}{2} \frac{1}{2} \frac{1}{2} \rangle$, where a is the lattice constant.

List True (T) or False (F)

- (ii) Dislocations are expected to glide parallel to {110} planes.

List True (T) or False (F)

- (iii) α Fe-C alloys are an example of substitutional solid solutions.

List True (T) or False (F)

3. This problem concerns bonding, structure and processing of thermoplastic polymers discussed in class.

a. Figure 9 shows the chemical formula and structure for polyethylene. Which of the following are true statements about the bonding in polyethylene.

i. The bonding within the chain is covalent

List True (T) or False (F)

ii. The bonding within the chain is characterized by sp^2 bonding

List True (T) or False (F)

iii. The bonding between chains is ionic due to electronegativity differences between the chains

List True (T) or False (F)

iv. The bonding between chains involves van der Waals bonding

List True (T) or False (F)

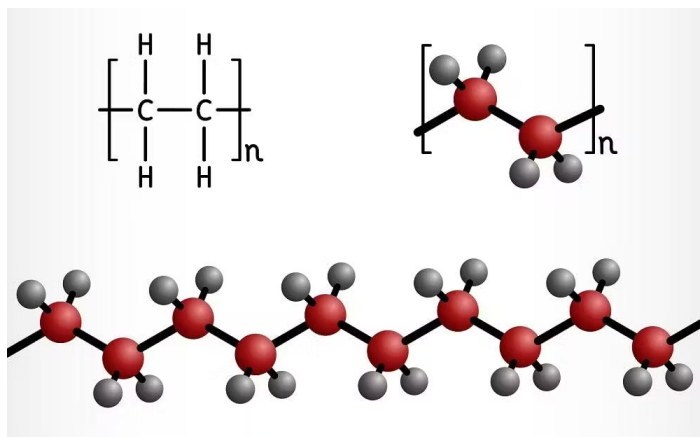


Figure 9: Chemical formula of polyethylene. Red and gray spheres are C and H, respectively.

Problem 3 Continues on the next page



- b. The top of Figure 10 below plots fraction transformed versus time for the crystallization of polypropylene from its melt (i.e., from an initial state with zero percent crystal phase). Polypropylene has a melting temperature of 180°C .
- Indicate on the upper plot the time for nucleation by circling the points corresponding to the start of nucleation at 160°C , 150°C and 140°C .
 - Plot the time for 50% transformation on the isothermal transformation (TTT) diagram in the lower panel of Figure 10, for 160°C , 150°C and 140°C .
 - Sketch a curve through these points on the TTT diagram and extend it to 60°C , showing a “nose” (corresponding to minimum transformation time) at 100°C .

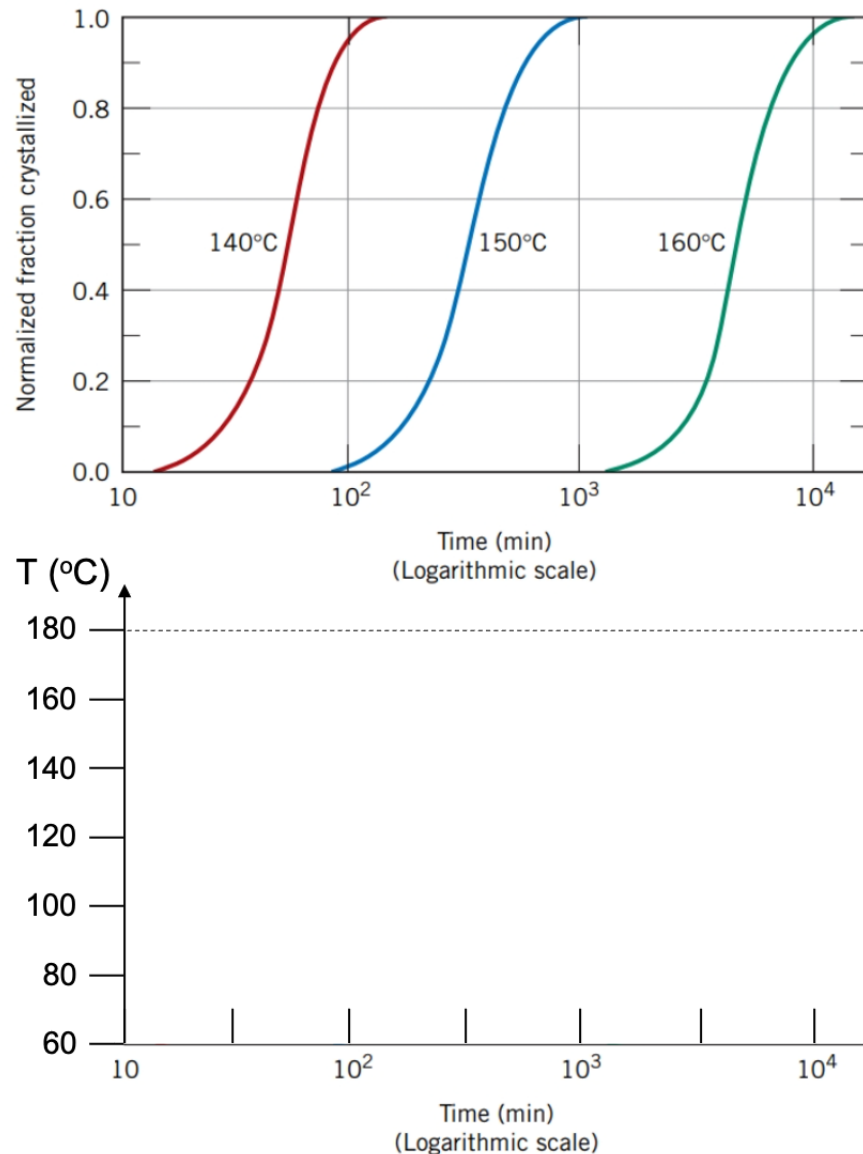


Figure 10: The top shows time for crystallization at three temperatures. The bottom is a TTT diagram for parts (ii) and (iii).

Problem 3 Continues on the next page



- c. Shown in Figure 11 is a characteristic microstructure of a semi-crystalline thermoplastic polymer, containing crystalline regions that have crystallized from the melt, and amorphous regions that represent untransformed liquid. Considering the information from Figure 10 in part (b), which one of the following three thermal paths would lead to the semicrystalline microstructure shown in Figure 11.
- Starting at 200°C, quench fast enough to avoid the nose in the TTT diagram, cooling below the glass transition temperature to create a frozen amorphous structure..
 - Starting at 200°C, quench to 140°C and hold for 10^3 minutes, and then quench to below the glass transition temperature.
 - Starting at 200°C, quench to 140°C and hold for 50 minutes, and then quench to below the glass transition temperature.

Answer (i, ii, or iii; there is only one correct answer):

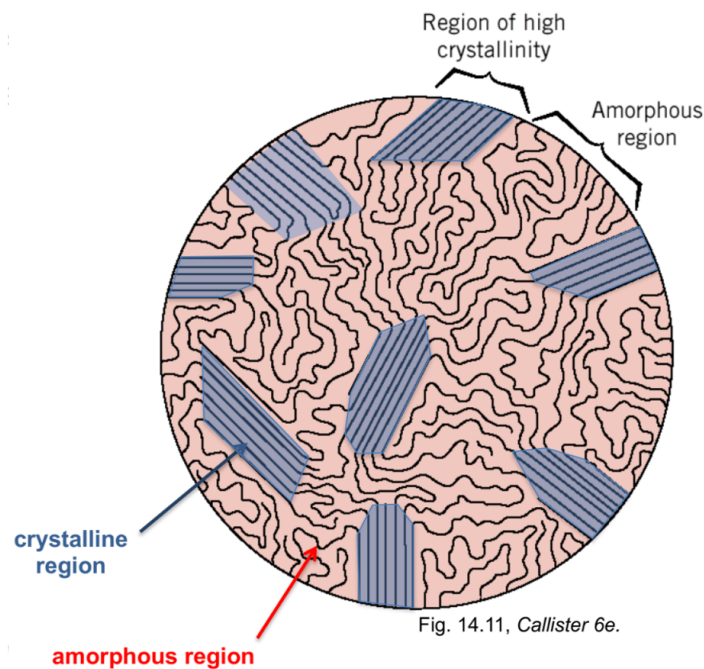


Figure 11: Semicrystalline polymer showing regions of crystal phase and regions of amorphous liquid/glass phase.

Problem 3 Continues on the next page



- d. The nose of a TTT diagram represents the minimum time we have to wait for nucleation. It occurs at a temperature where the nucleation rate ($\dot{N}$) is maximum. In class we wrote the nucleation rate as:

$$\dot{N} = K \left[\exp\left(-\frac{\Delta G^*}{kT}\right) \exp\left(-\frac{Q_d}{kT}\right) \right]$$

where the temperature (T) dependence is determined by the two exponential terms written in terms of the temperature-dependent free energy barrier for nucleation (ΔG^*) and the temperature-independent activation energy for diffusion (Q_d). Shown in Figure 12 is a plot of $\dot{N}$ for a phase transformation involving nucleation of a crystalline solid from the melt. The nucleation rate in Figure 12 is plotted as a function of temperature, and ΔT is the amount of undercooling below the melting temperature (T_m).

Also shown in Figure 12 by the dashed lines are the two exponential terms $\exp(-\Delta G^*/kT)$ and $\exp(-Q_d/kT)$, the product of which determines the temperature-dependence of the nucleation rate. From your knowledge of the temperature dependencies of these terms, write in the boxes in Figure 12 which dashed line corresponds to $\exp(-\Delta G^*/kT)$ and which corresponds to $\exp(-Q_d/kT)$.

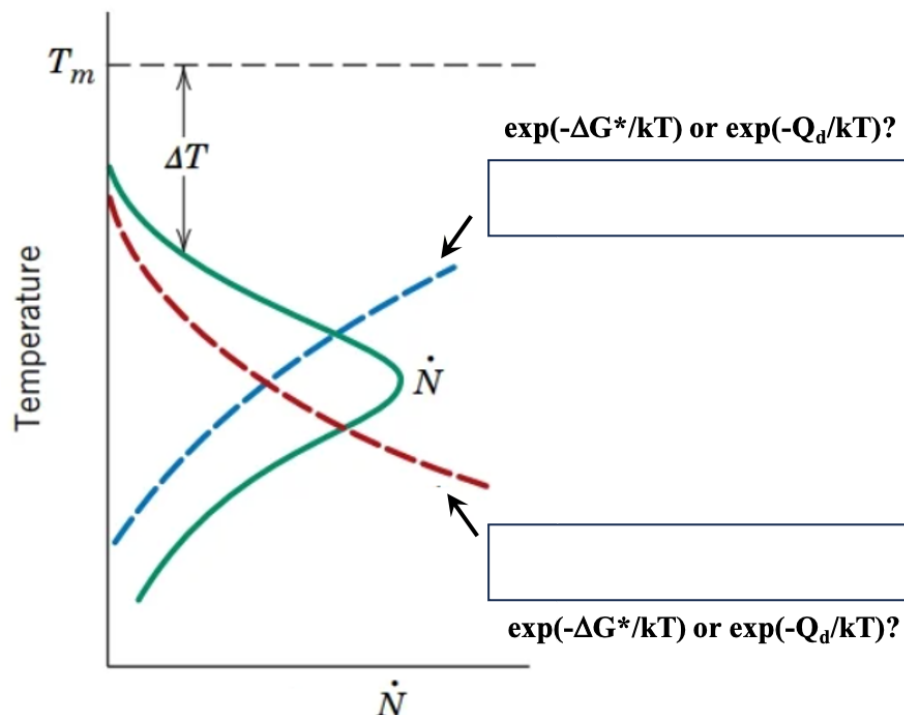


Figure 12: Nucleation rate versus temperature for nucleation of a crystalline solid from the melt.

4. This problem concerns electrical properties of materials.

- a. Copper is extensively used in engineering applications where we require wires with high electrical conductivity. Shown in Figure 13 on the next page is a plot of the electrical resistivity (ρ) of several copper-based metals versus temperature. The plot emphasizes that there are three distinct contributions to the resistivity $\rho = \rho_t + \rho_i + \rho_d$, where:

ρ_t is associated with temperature

ρ_i is associated with impurities, and

ρ_d is associated with deformation.

Recall that $\rho = 1 / \sigma$, where σ is the conductivity and $\sigma = n |e| \mu$ in terms of the carrier concentration (n) and mobility (μ). Given this information, and the data in Figure 13, answer the following questions (explanations are not required):

- i. Does the mobility (μ) decrease or increase as we raise the temperature for a material with constant composition and dislocation content?

Write “Increase” or “Decrease” based on which effect raising temperature has on value of μ

- ii. Recall that $\mu = |e| \tau / m$, where τ is the scattering time for electrons and m is electron mass. If deformation, temperature and solute additions do not change carrier concentration (n) or electron mass, which of the 5 materials shown in Figure 13 have maximum scattering time τ ?

Write “Pure”, “1.12 at.%Ni”, “Deformed”, “2.16 at.%Ni” or “3.32 at.%Ni” for the material in Figure 13 that has the maximum value of the scattering time τ .

- iii. Suppose that the deformation that produces the value of ρ_d shown in Figure 13 leads to the same increase in strength for copper as the addition of 2.16 at.% Ni. Which strategy should be used to produce wires with the highest yield strength and highest conductivity: strain hardening or solid-solution strengthening?

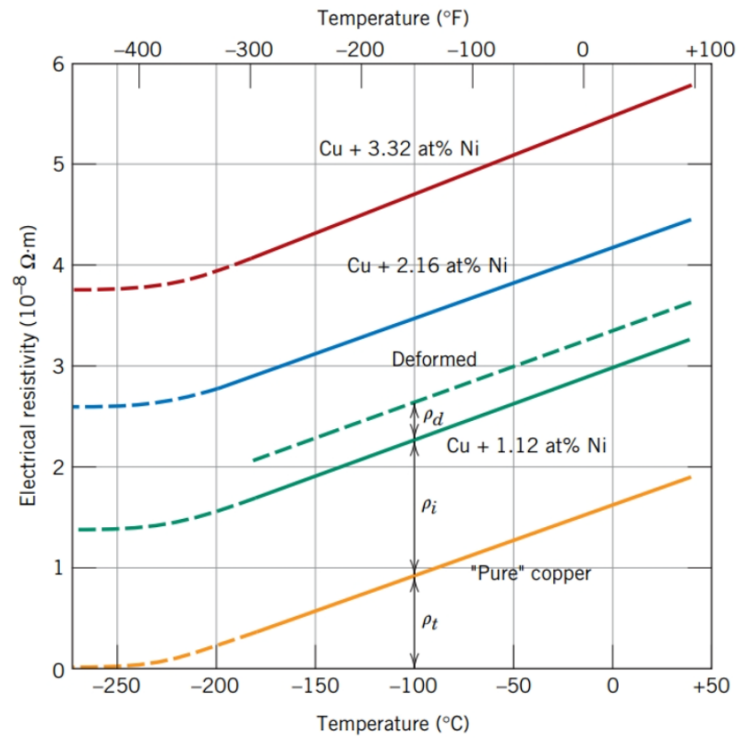
Write “Strain hardening” or “Solid-solution strengthening” based on which effect leads to higher strength and conductivity

Problem 4 Continues on the next page



Figure 13 The electrical resistivity versus temperature for copper and three copper–nickel alloys, one of which has been deformed. Thermal, impurity, and deformation contributions to the resistivity are indicated at -100°C .

[Adapted from J. O. Linde, *Ann. Physik*, **5**, 219 (1932); and C. A. Wert and R. M. Thomson, *Physics of Solids*, 2nd edition, McGraw-Hill Book Company, New York, 1970.]



Problem 4 Continues on the next page



- b. We will consider the effect on electrical conductivity of adding three different solute impurities to a Si semiconductor:

Impurity 1: Ge

Impurity 2: P

Impurity 3: B

Indicate below which impurity would give rise to the following measured effects, and briefly explain your answer in the space provided.

- i. It is measured that the conductivity in Si doped with this impurity decreases with increasing concentration of this impurity.

Write “Ge”, “P” or “B” based on which solute impurity gives rise to this measured effect

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Briefly explain your answer.

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- ii. It is measured that the concentration of holes in Si doped with this impurity to a concentration of 10^{21} m^{-3} is $p=10^{21} \text{ m}^{-3}$.

Write “Ge”, “P” or “B” based on which solute impurity gives rise to this measured effect

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Briefly explain your answer.

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- iii. It is measured at low temperatures that the concentration of electron carriers in Si doped with this impurity increases faster than the number of holes.

Write “Ge”, “P” or “B” based on which solute impurity gives rise to this measured effect

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Briefly explain your answer.

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Problem 4 Continues on the next page



- c. A Si semiconductor is doped with 10^{21} m^{-3} of Arsenic (As) donors. It shows extrinsic behavior for temperatures between 150 K to 450 K, and intrinsic behavior for above 450 K. Based on this and the information below, compute the conductivity at 300K and 900K. Show work leading to your answer in the space provided.
- The electron and hole mobilities in Si are $\mu_e=0.100 \text{ m}^2/\text{V-s}$ and $\mu_h=0.050 \text{ m}^2/\text{V-s}$, respectively, and you can assume these values are constant, independent of temperature.
 - The intrinsic concentration of electrons is $n_i = 10^{24} \text{ m}^{-3}$ at a temperature of 1000K.
 - Si has a bandgap of $E_{\text{gap}} = 1.11 \text{ eV}$.

Conductivity at 300 K (in $(\text{Ohm-m})^{-1}$ units to 3 sig figs)

Space for calculations:

Conductivity at 900 K (in $(\text{Ohm-m})^{-1}$ units to 3 sig figs)

Space for calculations:

Problem 4 Continues on the next page



- d. It is observed for the CaF_2 material considered in problem (1) that the total electrical conductivity (σ_{total}) is dominated by ionic conductivity (σ_{ionic}), i.e.: $\sigma_{\text{total}} = \sigma_{\text{ionic}}$. Recall from lecture that the mobility for ionic diffusion is given as $\mu_{\text{ionic}} = D_i / kT$, where D_i is the diffusion coefficient for ionic diffusion. For CaF_2 the relevant D_i is that associated with the F interstitial ions produced as Frenkel defects.

- i. Sketch the relation between $\ln(kT \cdot \sigma_{\text{total}})$ versus $1/T$ on the Arrhenius plot below.
- ii. In the box below specify if the negative of the slope of this plot is proportional to:

- (a) Q_m
- (b) Q_{fr}
- (c) $Q_m + \frac{1}{2} Q_{\text{fr}}$

where Q_{fr} is the formation energy of a Frenkel defect, and Q_m is the migration energy for F interstitial diffusion. Show your work that led to your answer in the space provided.

Answer in the box below (a), (b) or (c). There is only one correct answer.

Space for work:

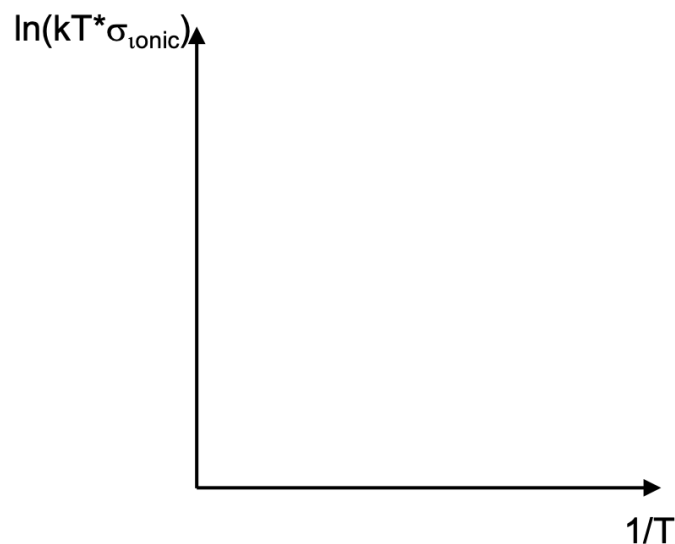


Figure 14: Arrhenius plot for problem 4.d.i.

5. **Extra credit.** You are asked to design a component requiring a material to have a high elastic stiffness. The component needs to have as small a mass as possible to optimize performance. Detailed design calculations determine that maximizing performance requires maximizing the quantity E / ρ where E is Young's modulus and ρ is mass density. The material currently being used for the application is carbon-fiber reinforced polymer (CFRP). From the Ashby plot below, we can see that all materials above the dashed line indicated will give performance equal to or better than CFRP.

One set of materials that could show higher performance is ceramics that are made of light elements, such as Al_2O_3 , B_4C , Si_3N_4 , and SiC . In this problem we will consider the reasons why these materials are good candidates, and why they have drawbacks.

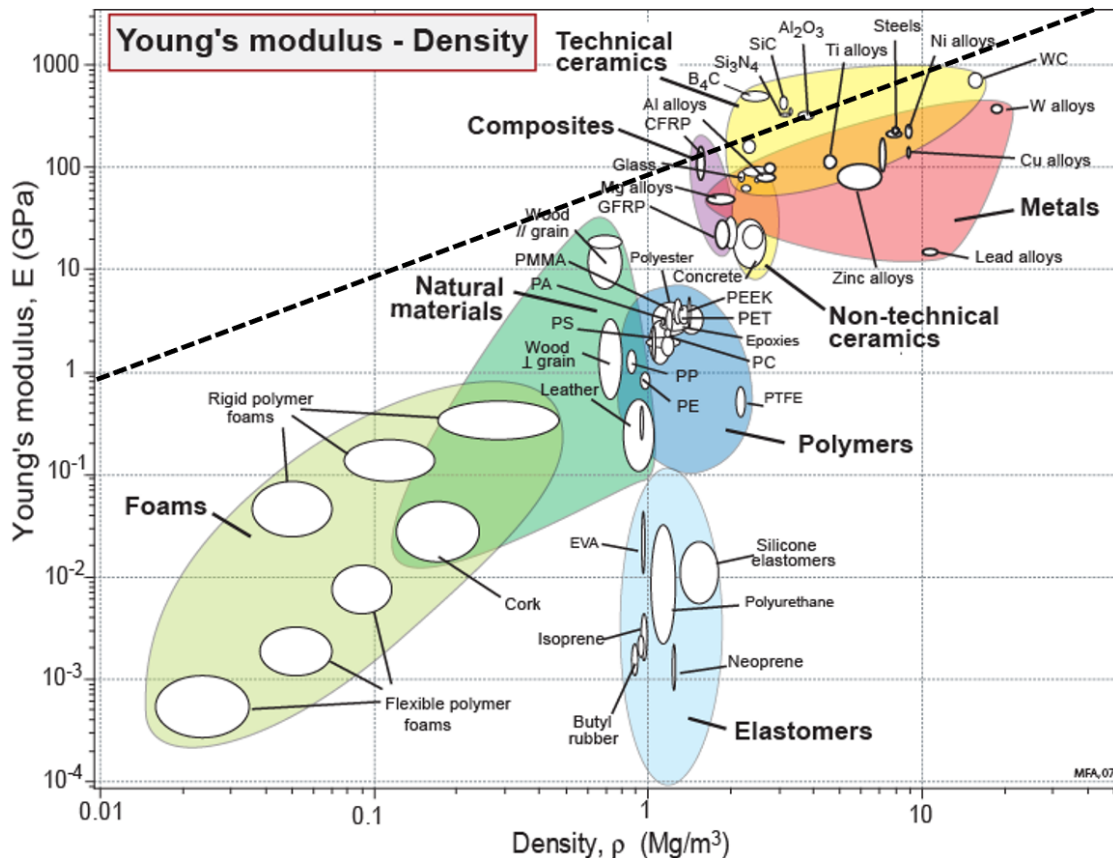


Figure 15: Ashby plot of Young's modulus versus density with a dashed line corresponding to constant values of E / ρ .

Problem 5 Continues on the next page



- a. Draw a schematic plot of energy and force versus bond length (r) for the bonds in any general material (not just those considered on the previous page) on Figure 16 below, and describe in words, in the box below it, what features of each curve determines the value of the elastic modulus.

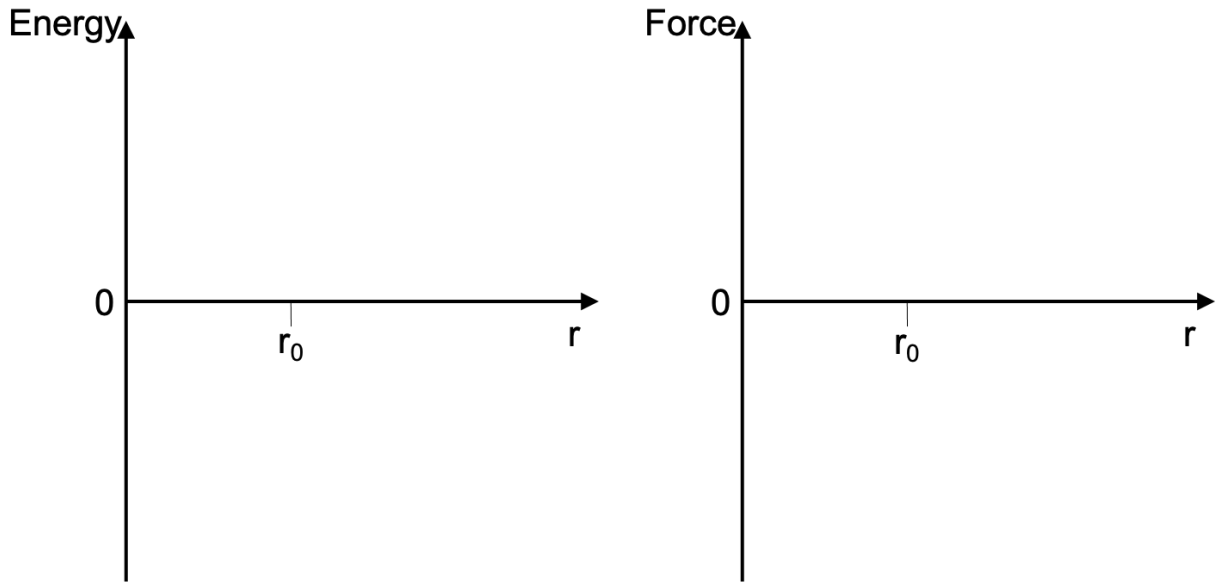


Figure 16: Plots on which to make the sketches for part (a).

Describe what features of the curves above determine the value of the elastic modulus

Problem 5 Continues on the next page



- b. What is the dominant type of bonding in ceramic materials and describe what are the characteristics of this type of bonding that enable ceramics to have high values of Young's modulus, based on your answer to part (a)?

What is the dominant type of bonding in ceramic materials?

Describe what are the characteristics of the bonding enabling ceramics to have Young's modulus

- c. One drawback to the ceramics listed above is that they can be expensive to manufacture. What is one other drawback of ceramics that would limit their application if we want to avoid catastrophic failure?

Space for your answer

Problem 5 Continues on the next page



- d. What are features of the bonding, structure, and deformation of metals that makes them have high fracture toughness, and thus might make them better candidates as materials for safety-critical applications? Address each point explicitly for full credit.

Space for your answer

END OF EXAM. NEXT PAGES ARE REFERENCE SHEETS.

Formulas, Constants, and Definitions

Constants and Units

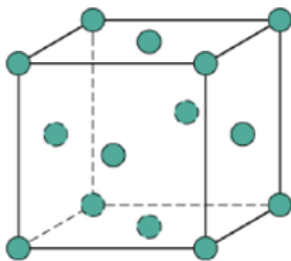
- *Boltzmann Constant*: $k = 1.3806 \times 10^{-23} \text{ J / K} = 8.6173 \times 10^{-5} \text{ eV / K}$
- *Avogadro's Number*: $N_A = 6.022 \times 10^{23} \text{ atoms / mol}$
- *Atomic Mass*: $1 \text{ amu} = 1 \text{ g / mol}$
- *Planck's Constant*: $h = 4.136 \times 10^{-15} \text{ eV s}$
- *Speed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

Bonding

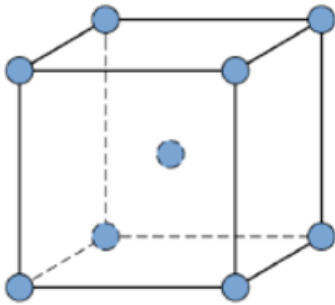
- *Types of Primary Bonding*: Ionic, Covalent, Metallic
- *Secondary Bonding*: Dipole-Dipole, Hydrogen, Dipole-Induced Dipole, Fluctuating Dipole

Crystallography

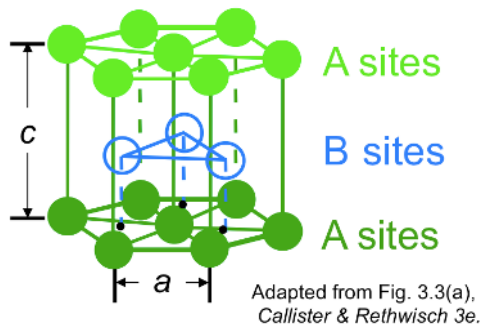
- *Bragg's Law*: $2 d_{hkl} \sin\theta = n \lambda$
- *Interplanar Spacing in Cubic Crystals*: $d_{hkl} = a / (h^2 + k^2 + l^2)^{1/2}$
- *FCC Structure (ABCABCABC...)*:



- *BCC Structure:*



- *HCP Structure (ABABAB...):*



- *Point Coordinates:* ijk
- *Crystallographic Directions:* $[ijk]$
- *Family of Crystallographic Directions:* $\langle ijk \rangle$
- *Miller Indices for Planes:* (hkl)
- *Family of Planes:* $\{hkl\}$

Defects

- *Point Defects:* Vacancies, Impurities, Interstitials, Schottky 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:* $N_v / N = \exp[-Q_v / kT]$
- *Equilibrium Concentration of Schottky Defects in a Metal Oxide:* $N_s / N = \exp(-Q_s / 2kT)$
- *Equilibrium Concentration of Frenkel Defects in a Metal Oxide:* $N_f / N = \exp(-Q_f / 2kT)$

Phase Diagrams

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

Kinetics

- *Temperature Dependence of Diffusion Constant:* $D = D_0 \exp[-Q_d / kT]$
- *Diffusion Activation Energy for Diffusion by vacancy mechanism:* $Q_d = Q_m + Q_v$
- *Diffusion Activation Energy for Diffusion by interstitial mechanism:* $Q_d = Q_m$

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

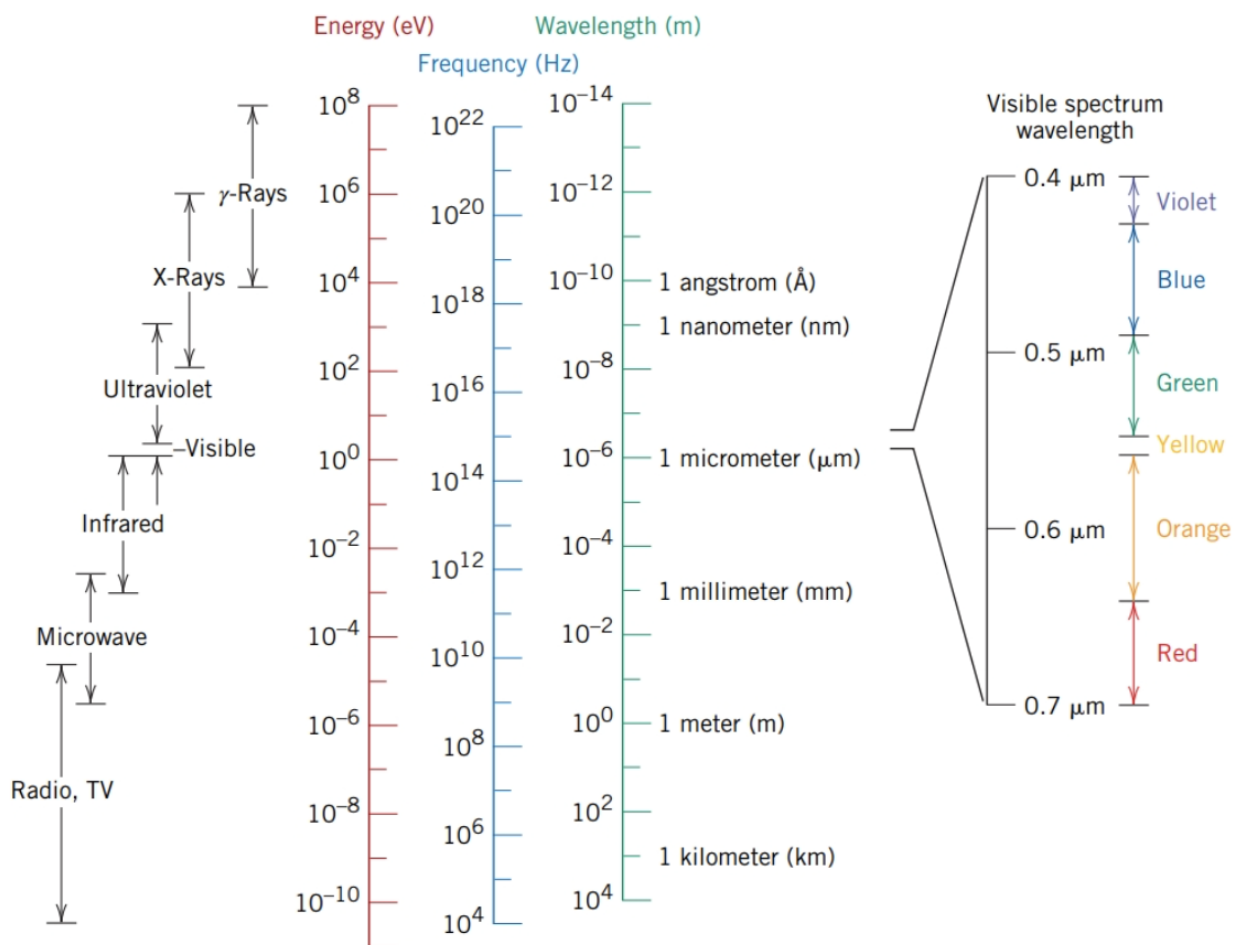
- *Conservation of Energy in terms of intensities of incident, reflected, absorbed, scattered and transmitted light intensities:* $I_0 = I_R + I_A + I_S + I_T$
- *Relationship Between Speed of Light, Wavelength (λ) and Frequency (ν):* $c = \lambda \nu$
- *Energy of Photon:* $E = h \nu$
- *Relationship Between Index of Refraction (n) and Dielectric Constant (ϵ_r):* $n^2 = \epsilon_r$
- *Snell's Law:* $n_1 \sin(\theta_1) = n_2 \sin(\theta_2)$
- *Reflectance (Fraction of Incident Light Reflected):* $R = [(n-1)/(n+1)]^2$

Mechanical Properties

- *Young's Modulus (E) in Linear Elastic Regime:* $\sigma = E \epsilon$
- *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 $\epsilon_p = 0.002$

- | | | | | | | | | | | | | | | | | | | | | | | | |
|-----------------|-----------------|----------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|---------------|-----------------|-----------------|----------------|----------------|-----------------|---------------|
| IA | | | | | | | | | | | | | | | | | | | | | | 0 | |
| 1
H
2.1 | | | | | | | | | | | | | | | | | | | | | | 2
He
- | |
| 3
Li
1.0 | IIA | | | | | | | | | | | | | | | | | IIIA | IVA | VA | VIA | VIIA | 10
Ne
- |
| 4
Be
1.5 | | | | | | | | | | | | | | | | | | 5
B
2.0 | 6
C
2.5 | 7
N
3.0 | 8
O
3.5 | 9
F
4.0 | 18
Ar
- |
| 11
Na
0.9 | 12
Mg
1.2 | | | | | | | | | | | | | | | | | 13
Al
1.5 | 14
Si
1.8 | 15
P
2.1 | 16
S
2.5 | 17
Cl
3.0 | 36
Kr
- |
| | | IIIB | IVB | VB | VIB | VIIB | VIII | | | IB | IIB | | | | | | 35
Br
- | | | | | | |
| 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 | 54
Xe
- | | | | | | |
| 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 | 86
Rn
- | | | | | | |
| 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 | | | | | | | |
| 87
Fr
0.7 | 88
Ra
0.9 | 89-102
Ac-No
1.1-1.7 | | | | | | | | | | | | | | | | | | | | | |

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Electromagnetic Spectrum. Reproduced from Callister.

COLOR	WAVELENGTH	ENERGY
Red	700 nm	1.771 eV
Reddish orange	650 nm	1.909 eV
Orange	600 nm	2.067 eV
Yellow	580 nm	2.138 eV
Yellowish green	550 nm	2.254 eV
Green	500 nm	2.480 eV
Blue	450 nm	2.765 eV
Violet	400 nm	3.100 eV

Wavelengths and energy of visible light (from K.Nassau, "Experimenting with Color")