Chapter 1 Supplemental Problems

1. Lead is FCC and its atomic radius is 1.746×10^{-8} cm. What is the volume of its unit cell?

2. Silver has a face-centered cubic structure with a lattice constant of 4.077 Å. Its atomic weight is 107.88 g/mol. Calculate the density of silver.

3. Zinc has a HCP structure. The height of the unit cell is 4.935 Å. The centers of the atoms in the base of the unit cell are 2.66 Å apart. (a) How many atoms are there per hexagonal unit cell? (Show reasoning.) (b) What is the volume of the hexagonal unit cell? (c) Would the calculated density be greater or less than the true density of 7.135 g/cc? (Justify your answer.)

4. Sodium and chlorine weigh 22.997 and 35.457 g/mol, respectively. If the density is 2.165 g/cc, calculate the dimensions of the unit cell of NaCl.

5. Calculate the lattice constant of the unit cell of iron (BCC) from the atom size.

6. Show in tabular form the relationship between atoms size (r) and unit cell dimensions for FCC, BCC, and simple cubic structure.

	FCC	BCC	SC
Side of unit cell			
Face diagonal			
Body diagonal			

7. What is the coordination number of copper in a face-centered cubic structure?

8. An alloy contains 85 wt% copper and 15 wt% tin. Calculate the atomic percent of each element.

9. 5 atomic % magnesium is present in an Al-Mg alloy. Calculate the weight percent magnesium.

10. Iron is changed from BCC to FCC. What is the percent volume change? (Radii for BCC and FCC iron are 1.238 and 1.27 Å, respectively.)

11. If 1.0% carbon, by weight, is present in a face-centered cubic iron, what percent of the unit cells will have carbon atoms?

12. Calculate the minimum potential energy (in KJ/mol) and the maximum force (in N) for the ionic pair Na^+-Cl^-. The interionic equilibrium distance r_o = 2.36 Å,.

13. X-rays with a wavelength of 0.58 Å are used for calculating $d_{(200)}$ in nickel. The reflection angle is 9.5°. What is the size of the unit cell?

14. The lattice constant for a unit cell of aluminum is 4.041 Å. (a) What is $d_{(220)}$? (b) $d_{(111)}$)? (c) $d_{(200)}$?

15. (a) How many atoms are there per square millimeter on a (100) plane of copper? (b) (110) plane? (c) (111) plane?

16. Nickel is face-centered cubic with an atomic radius of 1.243 Å. (a) What is the spacing between the (200) planes? (b) between the (220) planes? (c) between the (111) planes?

17. A sodium chloride crystal is used to measure the wavelength of some x-rays. The diffraction angle is 5.2° for the (111) spacing of the chlorine. What is the wavelength? (The lattice constant is 5.63 Å.)

18. The distance between (110) planes in a body-centered cubic structure is 2.03 Å. (a) What is the size of the unit cell? (b) What is the radius of the atoms? (c) What might the metal be?

19. Calculate the radius of the largest atom which can be located in the interstices of body-centered iron without crowding (Hint: Sketch the (100) face of several adjacent unit cells.)

20. Determine the radius of the largest atom which can be located in the interstices of BCC iron without crowding (Hint: The center of the largest hole is located at a/2, b/4, c=0.)
21. Consider a mixture of 10 mol% Na_2O, 10 mol% Al_2O_3 and the balance SiO_2. Identify the glass former, the intermediate and the modifier in the mixture. What type of silicate network will be formed?
22. A sample of polystyrene has a weight-average molecular weight of 3.3×10^6. If the polydispersity index is 1.5, what is the average degree of polymerization for the sample?
23. The number average molecular weight of polypropylene is 1,000,000 g/mol. Compute the number-average degree of polymerization.
24. Polyester is formed from the reaction of a diol with a diacid. Is the polymer structure linear, branched or network? If glycol $C_3H_5(OH)_3$ is added to the polymerization mixture, does the structure change, and if so, how? Comment on how the ability of the polymer to crystallize might change upon addition of glycol.

Answers

1) 121 Å^3. 2) 10.58 g/cc
3) (a) 6; (b) 9.05×10^{-23} cm^3, (c) 7.17 g/cc (this makes no allowance for imperfections.)
4) 5.63×10^{-8} cm. 5) 2.86 Å.
6)

	FCC	BCC	SC
Side	$4r/\sqrt{2}$	$4r/\sqrt{3}$	2r
Face diagonal	4r	$\sqrt{2/3}(4r)$	$\sqrt{2}(2r)$
Body diagonal	$(4r)/\sqrt{2/3}$	4r	$\sqrt{3}(2r)$

7) 12 8) 8.7 atomic% Sn, 91.3 at% Cu. 9) 4.5% Mg. 10) 0.9% contraction
11) 19% of unit cells have carbon. 12) $U_{min} = 514$ KJ/mol, $F_{max} = 4 \times 10^{-9}$ N
13) 3.52 Å 14) (a) 1.43 Å; (b) 2.33 Å; (c) 2.02 Å 15) (a) 1.535×10^{13} atoms/mm^2; (b) 1.0854×10^{13} atoms/mm^2; (c) 1.77×10^{13} atoms/mm^2 16) (a) 1.76 Å; (b) 1.243 Å (4 spacings per face diagonal); (c) 2.04 Å (3 spacings per body diagonal) 17) 0.59 Å 18) (a) 2.86 Å; (b) 1.24 Å; (c) BCC iron, or Cr (not Ni). 19) 0.525 Å 20) 0.37 Å 21) SiO_2 is the glass former, Al_2O_3 is the intermediate and Na_2O is the modifier. The O/Si ratio is 2.5, so sheet silicates will result. 22) 21,154 23) 23,810 24)Linear. Addition of glycol causes branching and possibly network formation. This branching inhibits crystallization due to steric hindrance.

Thought Problems/Review Questions
1. Draw an electron energy diagram for an atom as a function of distance to another atom.
2. What are hybrid energy bonds? Why are they important in bonding?
3. Draw a potential energy function for two atoms as they approach one another.
4. Is the potential energy function spherically symmetric? Why?
5. What is the significance is the width of the potential energy well?
6. Explain how the differences in electronegativities of the elements affects the potential energy function. Why would Xe react with fluorine and not nitrogen?
7. What is an alloy?
8. What major alloying element is used in stainless steels? Why?
9. What are the Hume-Rothery rules for formation of alloys?
10. Account for the following fact: H_2O and HF have much higher boiling points (100 and 19.4°C, respectively) than H_2S and HCl (-60.7 and -85° C, respectively) although the molecular weight of H_2O and HF is lower than that of H_2S and HCl.
11. If the hydrogen 1s and fluorine 2p atomic orbitals were by some process made equal in energy, what effect would this have on the character of the bond in HF?
12. Each boron atom has three valence electrons. Why is the B_2 molecule not held together by a triple bond as N_2 is?
13. Which of the following molecules are paramagnetic: CO, Cl_2, NO, N_2?
14. Define the following: coordination polyhedra; unit cell; Miller indices; Miller-Bravais indices.
15. How are the Miller indices applied to interpreting X-ray diffraction images of a solid?

16. How can one interpret crystal structure from X-ray or electron diffraction images?
17. What is a glass-ceramic?
18. Why are there generally two quoted values of molecular weight for synthetic polymers? What significance is their ratio?
19. What effect would the addition of large, bulky groups in the chain or along the side of the chain have on the melting point and glass transition temperature of a polymer?
20. What are the thermoset resins which are normally used in reinforced plastics?
21. What are the thermoplastic resins which are usually used in reinforced plastics?
22. Why do you think that fibers or whiskers increase the load bearing ability of a matrix?
23. Besides the choice of matrix and reinforcing agent, what other additives could be utilized?
24. What is a coupling agent and what purpose does it serve?
25. What are the major types of glasses used in glass fiber reinforced plastics (GFRP)?
26. Sketch the chain architecture (configuration) of a typical block copolymer.
27. Write out the structural formulas of the following common synthetic polymers: polystyrene, polyethylene, polypropylene, polyvinylchloride, polymethacrylate, polymethyl methacrylate, polybutadiene, polyisoprene, polytetrafluoroethylene, polyvinylidene fluoride, ABS resin, polyacrylonitrile, polyethylene terphthalate.