



Do yourself a solid.

3.091: Introduction to Solid State Chemistry
Fall 2018

Practice Problems F: Electronic materials and crystallography

The following problems sets are compiled from B. A. Averill and P. Eldredge, *General Chemistry: Principles, Patterns, and Applications*. License: CC BY-NC-SA. Source: [Open Textbook Library](#).

Reading: Averill 12.6.1-12.6.4; 12.1-12.3

1. Charge carrier density

Chemical analysis of a germanium crystal reveals indium at a level of 0.0003 atomic percent.

- Assuming that the concentration of thermally excited charge carriers from the Ge matrix is negligible, calculate the density of free charge carriers (carriers/cm³) in this Ge crystal.
- Draw a schematic energy band diagram for this material and label all critical features.

2. Band gap ↔ wavelength

Show that green light ($\lambda = 5 \times 10^{-7}m$) can excite electrons across the band gap of silicon (1.14 eV).

3. Substitutional doping concentration

Determine the amount (in grams) of arsenic required to be substitutionally incorporated into a mmole of silicon in order to achieve a free electron density of $5 \times 10^{17}/cm^3$ in it.

4. Density of free charge carriers

- Chemical analysis of a silicon crystal reveals arsenic at a level of 0.0002 atomic percent. Assuming that the concentration of thermally excited charge carriers from the Si matrix is negligible, calculate the density of free charge carriers (carriers/cm³) in this Si crystal.
- Draw a schematic energy band diagram for this material, and label all critical features.

5. Charge carrier density

Determine the amount (in grams) of boron that must be substitutionally incorporated into 1 kg of germanium to establish a charge carrier density of $3.091 \times 10^{17}/cm^3$

6. Incident beam energy from electron velocity

- An electron beam strikes a crystal of cadmium sulfide (CdS). Electrons scattered by the crystal move at a velocity of 4.4×10^5 m/s. Calculate the energy of the incident beam. Express your result in eV. CdS is a semiconductor with a band gap $E_g=2.45eV$.
- Cadmium telluride (CdTe) is also a semiconductor. Do you expect the band gap of this material to be greater or less than the band gap of CdS? Explain.



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7. Absorption spectra and periodic trends

- Aluminum phosphide (AlP) is a semiconductor with a band gap, E_g , of 3.0 eV. Sketch the absorption spectrum of this material, i.e. plot % absorption vs wavelength λ .
- Aluminum antimonide (AlSb) is also a semiconductor. Do you expect the band gap of this material to be greater than or less than the band gap of AlP? Explain.

8. n-type doping

You wish to make n-type germanium.

- Name a suitable dopant.
- Name the majority charge carrier in the doped material.
- Draw a schematic energy band diagram of the doped material. Label the valence band, conduction band, and any energy levels associated with the presence of the dopant.

9. Unit cells

Averill Chapter 12, Section 2, Conceptual Problem 1

Why is it valid to represent the structure of a crystalline solid by the structure of its unit cell? What are the most important constraints in selecting a unit cell?

10. Packing efficiency

Averill Chapter 12, Section 2, Conceptual Problem 8

Arrange the three types of cubic unit cells in order of increasing packing efficiency. What is the difference in packing efficiency between the hcp structure and the ccp structure?

11. Structure under pressure

Averill Chapter 12, Section 2, Conceptual Problem 9

The structures of many metals depend on pressure and temperature. Which structure- bcc or hcp- would be more likely in a given metal at very high pressures? Explain your reasoning.

12. Structure and density

Averill Chapter 12, Section 2, Numerical Problem 3

The density of nickel is 8.908 g/cm³. If the metallic radius of nickel is 125 pm, what is the structure of metallic nickel?



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13. Structure and density

Averill Chapter 12, Section 2, Numerical Problem 5

An element has a density of 10.25 g/cm^3 and a metallic radius of 136.2 pm . The metal crystallizes in a bcc lattice. Identify the element.

14. Structure and density

Averill Chapter 12, Section 2, Numerical Problem 9

Lithium crystallizes in a bcc structure with an edge length of 3.509 \AA . Calculate its density. What is the appropriate metallic radius of lithium in picometers?

15. SC vs BCC

Averill Chapter 12, Section 3, Conceptual Problem 4

The unit cell of cesium chloride consists of a cubic array of chloride ions with a cesium ion in the center. Why then is cesium chloride described as having a simple cubic structure rather than a bcc structure? The unit cell of iron also consists of a cubic array of iron atoms with an iron atom in the center of the cube. Is this a bcc or a simple cubic unit cell? Explain your answer.

16. Density, temperature, and structure

Iron ($\rho = 7.69 \text{ g/cm}^3$) crystallizes in a bcc unit cell at room temperature. Calculate the radius of an iron atom in this crystal. At temperatures above 910°C , iron prefers to be fcc. If the temperature dependence of the radius of the iron atom is negligible, calculate the density of the fcc iron. Use this to determine whether iron expands or contracts when it undergoes transformation from the bcc to fcc structure.

17. Interplanar spacing and distance to second-nearest neighbors

For the element copper, determine:

- The distance of second nearest neighbors; and
- The interplanar spacing of 110 planes

18. Directions in a crystallographic plane

Consider a (111) plane in an FCC structure. How many different [110]-type directions lie in this (111) plane? Write out the indices for each such direction.



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19. Planar packing fraction

For aluminum at 300K, calculate the planar packing fraction (fractional area occupied by atoms) of the (110) plane.

20. Lattice points along crystallographic directions

Shackelford, Introduction to Materials Science for Engineers, Chapter 3, Problem 3.9

Which lattice points lie on the $[110]$ direction in the FCC unit cell?

21. Members of a crystallographic family of directions

Shackelford, Introduction to Materials Science for Engineers, Chapter 3, Problem 3.10

List the members of the $\langle 110 \rangle$ family of directions in the cubic system.

22. Members of a crystallographic family of planes

Shackelford, Introduction to Materials Science for Engineers, Chapter 3, Problem 3.13

List the members of the 110 family of planes in the cubic system.

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