3.091: Introduction to Solid State Chemistry
Fall 2018
Practice Problems H: Defects

Reading: Averill 12.4.4-12.4.5; supplemental reading (posted)

1. Covalent solids under stress

Averill Chapter 12, Section 4, Conceptual Problem 2

Why does applying a mechanical stress to a covalent solid cause it to fracture? Use an atomic level description to explain why a metal is ductile under conditions that cause a covalent solid to fracture.

2. Work hardening

Averill Chapter 12, Section 4, Conceptual Problem 3

How does work hardening increase the strength of a metal? How does work hardening affect the physical properties of a metal?

3. Crack formation

Averill Chapter 12, Section 4, Conceptual Problem 4

Work-hardened metals and covalent solids such as diamonds are both susceptible to cracking when stressed. Explain how such different materials can both exhibit this property.

4. Ductility

Averill Chapter 12, Section 4, Conceptual Problem 5

Suppose you want to produce a ductile material with improved properties. Would impurity atoms of similar or dissimilar atomic size be better at maintaining the ductility of a metal? Why? How would introducing an impurity that forms polar covalent bonds with the metal atoms affect the ductility of the metal? Explain your reasoning.

5. Substitutional vs. interstitial impurities

Averill Chapter 12, Section 4, Conceptual Problem 6

Substitutional impurities are often used to tune the properties of the material. Why are substitutional impurities generally more effective at high concentrations, whereas interstitial impurities are usually effective at low concentrations?

6. Properties of a substitutional impurity

Averill Chapter 12, Section 4, Conceptual Problem 7

If an O^{2-} ion (ionic radius = 132 pm) is substituted for an F^{-} ion (ionic radius = 133 pm) in an ionic crystal, what structural cahnges in the ionic lattice will result?

7. Charged impurity

Averill Chapter 12, Section 4, Conceptual Problem 8

How will the introduction of a metal ion with a different charge as an impurity induce the formation of oxygen vacancies in an ionic metal-oxide crystal?

8. Making oxygen vacancies

Averill Chapter 12, Section 4, Conceptual Problem 10

If you wanted to induce the formation of oxygen vacancies in an ionic crystal, which would you introduce as substitutional impurities- cations with a higher positive charge or a lower positive charge than the cations in the parent structure? Explain your reasoning.

9. Substituting K^{+} for Na^{+}

Averill Chapter 12, Section 4, Numerical Problem 1

The ionic radius of K^{+} is 133 pm, whereas that of Na^{+} is 98 pm. Do you expect $K^{=}+$ to be a common substitutional impurity in compounds containing Na^{+}? Why or why not?

10. Choose the most likely interstitial

Averill Chapter 12, Section 4, Numerical Problem 2

Given Cs (262 pm) Tl (171 pm), and B (88 pm) with their noted atomic radii, which tom is most likely to act as an interstitial impurity in an Sn lattice (Sn atomic radius = 144 pm)? Why?

11. Generating oxygen vacancies via doping

Averill Chapter 12, Section 4, Numerical Problem 4

Certain ceramic materials are good electrical conductors due to high mobility of oxide ions resulting from the presence of oxygen vacancies. Zirconia (ZrO_2) can be doped with yttrium by adding Y_2O_3. If 0.35 g of Y_2O_3 can be incorporated into 25.0 g of ZrO_2 while maintaining the zirconia structure, what is the percentage of oxygen vacancies in the structure?

12. Choose the best ion to make an oxygen vacancy

Averill Chapter 12, Section 4, Numerical Problem 5

Which of the following ions is most effective at inducing an O^{2-} vacancy in crystalline CaO? The ionic radii are O^{2-}, 132 pm; Ca^{2+}, 100 pm; Sr^{2+}, 127pm; F^{-}, 133pm; La^{3+}, 104 pm; and K^{+}, 133 pm. Explain your reasoning.

13. Calculate vacancy fraction given temperature

Calculate the vacancy fraction in copper at (i) 20°C and (ii) the melting point, 1085°C. Measurements have determined the values of the enthalpy of vacancy formation, ΔH_v, to be 1.03 eV and the entropic prefactor, A, to be 1.1.

14. Enthalpy of vacancy formation given vacancy fraction at two temperatures

In iridium (Ir), the vacancy fraction, $\frac{n_v}{N}$ is 3.091×10^{-5} at 1234°C and 5.26×10^{-3} at the melting point. Calculate the enthalpy of vacancy formation, ΔH_v.

15. Using an initial condition to calculate vacancy concentration

A formation energy of 2.0 eV is required to create a vacancy in a particular metal. At 800°C there is one vacancy for every 10,000 atoms.

a) At what temperature will there be one vacancy for every 1,000 atoms?

b) Repeat the calculation, but this time with an activation energy of 1.0 eV. Note the big change in the temperature interval necessary to obtain the same change in vacancy concentration as was the case with an activation energy of 2.0 eV.

16. Relating materials properties to types of defects

Identify 3 types of crystal defects in solids (one point, one linear, and one planar) and suggest for each of these one material property that is adversely affected by its presence and one that is improved. Also state what to look for in a crystal that possesses each of these defects.

17. Slip directions along a plane

Identify the directions of slip for indium (FCC) on the (111) plane.