

HOMework 5.

solutions



Textbook Problems: Imperfections in Solids

1. Askeland 4-67. Why is most “gold” or “silver” jewelry made out of gold or silver alloyed with copper, i.e, what advantages does copper offer?

We have two major considerations in jewelry alloying: strength and cost. Copper additions obviously lower the cost of gold or silver (Note that 14K gold is actually only about 50% gold). Copper and other alloy additions also strengthen pure gold and pure silver. In both gold and silver, copper will strengthen the material by either solid solution strengthening (substitutional Cu atoms in the Au or Ag crystal), or by formation of second phase in the microstructure.

2. Solid state solubility. Of the elements in the chart below, name those that would form each of the following relationships with copper (non-metals only have atomic radii listed):
- Substitutional solid solution with complete solubility
 - Ni and possibly Ag, Pd, and Pt
 - Substitutional solid solution of incomplete solubility
 - Ag, Pd, and Pt (if you didn't include these in part (a); Al, Co, Cr, Fe, Zn)
 - An interstitial solid solution
 - C, H, O (small atomic radii)

Element	Atomic Radius (nm)	Crystal Structure	Electronegativity	Valence
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Pt	0.1387	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

3. Vacancies. Calculate the fraction of atom sites that are vacant for pure lead at room temperature (25 °C) and at 310 °C (just below its melting temperature). The activation energy for vacancy formation is about 53 kJ/mole. How do you think the difference in the fraction of vacant sites will affect self-diffusion (diffusion of the atoms within their own crystal)?

The fraction of vacant sites is given by the following expression:

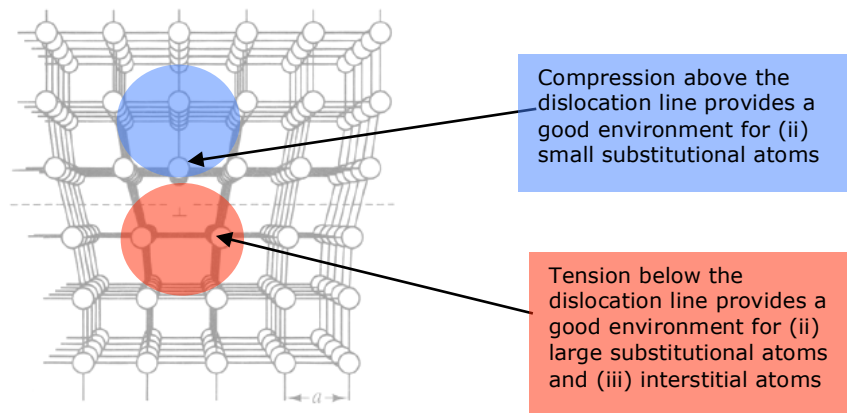
$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

Note that k , the Boltzmann constant, is used for activation energies given per atom. The gas constant R is used with activation energies given on a mole basis. We'll need to use R for this problem. The fractions of vacant sites for the two temperatures are as follows:

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{RT}\right) = \exp\left(\frac{-53,000\text{J/mole}}{(8.31\text{J/moleK})(298\text{K})}\right) = 5.1 \times 10^{-10}$$

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{RT}\right) = \exp\left(\frac{-53,000\text{J/mole}}{(8.31\text{J/moleK})(583\text{K})}\right) = 1.8 \times 10^{-5}$$

4. Strain fields around dislocations. Sketch the distortion of a crystal lattice around an edge dislocation, and show the preferred regions for (i) large substitutional atoms, (ii) small substitutional atoms, and (iii) interstitial atoms. HINT: Determine the type of distortion (tension or compression) that the large and small substitutional atoms will have on a perfect lattice, then think of how the distortion around a dislocation could best be balanced or relieved by the distortion caused by the substitutional atoms.



Open-Ended Problem: Imperfections in Solids

1. Askeland Problems 2-38 and 21-31. *NOTE: Only one answer is required, as they are very similar problems.*
 (2-38) Turbine blades used in jet engines can be made from such materials as nickel-based superalloys. We can, in principle, even use ceramic materials such as zirconia or other alloys based on steels. In some cases, the blades also may have to be coated with a thermal barrier coating (TBC) to minimize exposure of the blade material to high temperatures. What design parameters would you consider in selecting a material for the turbine blade and for the coating that would work successfully in a turbine engine? Note that different parts of the engine are exposed to different temperatures, and not all blades are exposed to relatively high temperatures. What problems might occur? Consider the factors such as temperature and humidity in the environment that the turbine blades must function.

(21-31) What design constraints exist in selecting materials for a turbine blade for a jet engine that is capable of operating at high temperatures?

Design parameters for turbine blades and protective coatings...here are some things that come to mind:

- Strength: Many turbine blades are subjected to high rotational speeds, so strength (particularly along the long axis) is a very important consideration.
- Melting temperature: Obviously, if the turbine blade and coating are subjected to high temperatures, we need materials with high melting points. Aluminum isn't going to cut it.
- High temperature strength: Not only do we need high strength, but we need to retain the high strength at high operating temperatures. Note that many materials have high strength values at room temperatures, but they become rather weak at elevated temperatures. Ever heard of creep? Creep, as defined in a materials science context, is deformation that occurs with elevated temperatures and stress.

- Coefficient of thermal expansion: Temperature cycling will cause thermal expansion of the turbine blade and connected components. We need to consider the dimensional changes that occur as temperatures are increased and decreased. Of particular importance are the differential changes in temperature between the turbine blade material and the materials used as coatings or those connected to the turbine blades. Differential expansion rates lead to thermally-induced stresses.
- Ductility and toughness: Turbine blades are often impacted by flying debris, including birds (ever heard of the frozen chicken test?). If this occurs, we don't want the turbine blade to catastrophically fail in a brittle manner...brittle failure at 30,000 feet...yikes! We'd much rather replace dented or bent blades that make it safely back down to the ground.
- Corrosion resistance: As the problem statement mentioned, we'll have to deal with temperature and humidity, not to mention salt spray if we're near the coast or flying over the ocean. Low alloy steel isn't going to cut it.
- Other stuff: Presence of defects/uniformity of material – we want a material that won't provide any microstructural surprises. Fatigue resistance may be important, depending on the frequency and amplitude of speed changes or on/off cycling. Wear resistance – again...flying debris.

Textbook Problems: Diffusion

1. Let's harden some steel by adding carbon near the surface! A carburizing process is carried out on a 0.10% C steel by introducing 1.0% C at the surface at 980 °C. At this temperature, the iron has a face-centered cubic (fcc) crystal structure. Calculate the carbon content at 0.01 cm, 0.05 cm, and 0.10 cm beneath the surface after 1 h, and plot these values on a graph of carbon composition versus position (distance into the steel). Assume that the carbon content at the surface remains constant.

IMPORTANT NOTE: The following solution is based on constant values found in the Askeland textbook, and the units found in Askeland (Q is in cal/mol, and D_0 is in cm^2/s). If you are using Callister for this problem, your values will be a bit different. For example, the Q value in Callister is 148,000 J/mol, which is equivalent to 35,400 cal/mole.

- 5–66** A carburizing process is carried out on a 0.10% C steel by introducing 1.0% C at the surface at 980°C, where the iron is FCC. Calculate the carbon content at 0.01 cm, 0.05 cm, and 0.10 cm beneath the surface after 1 h.

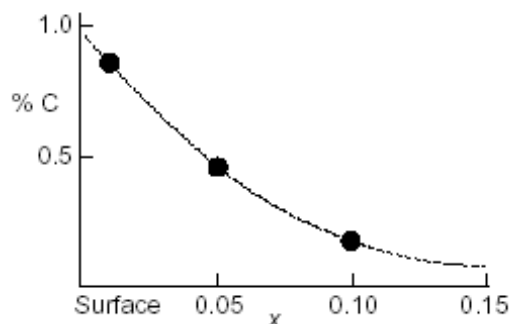
Solution: $D = 0.23 \exp[-32,900/(1.987)(1253)] = 42 \times 10^{-8} \text{ cm}^2/\text{s}$

$$\frac{1 - c_x}{1 - 0.1} = \text{erf}[x / (2\sqrt{(42 \times 10^{-8})(3600)})] = \text{erf}[x / 0.0778]$$

$$x = 0.01: \text{erf}[0.01/0.0778] = \text{erf}(0.1285) = \frac{(1 - c_x)}{0.9} = 0.144 \quad c_x = 0.87\% \text{ C}$$

$$x = 0.05: \text{erf}[0.05/0.0778] = \text{erf}(0.643) = \frac{(1 - c_x)}{0.9} = 0.636 \quad c_x = 0.43\% \text{ C}$$

$$x = 0.10: \text{erf}[0.10/0.0778] = \text{erf}(1.285) = \frac{(1 - c_x)}{0.9} = 0.914 \quad c_x = 0.18\% \text{ C}$$



2. Diffusivity. Values for the diffusion of carbon in bcc and fcc iron are given in the following table:

Materials	D_0 (cm ² /sec)	Q_d (kJ/mole)
C in bcc Fe	0.0079	83
C in fcc Fe	0.21	141

a. Calculate the diffusion coefficients for C in both fcc and bcc iron at 900 °C.

$$D = D_0 \exp\left(\frac{-Q_d}{RT}\right)$$

$$D_{fcc} = (0.21 \text{ cm}^2/\text{sec}) \exp\left(\frac{-141 \text{ kJ/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1173 \text{ K})}\right) = 1.10 \times 10^{-7} \text{ cm}^2/\text{sec}$$

$$D_{bcc} = (0.0079 \text{ cm}^2/\text{sec}) \exp\left(\frac{-83 \text{ kJ/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1173 \text{ K})}\right) = 1.58 \times 10^{-6} \text{ cm}^2/\text{sec}$$

b. Explain why you think the values are different.

The diffusivity of C is higher in bcc iron due to lower atomic packing and more interstitial void space compared to the fcc structure. More space leads to easier interstitial impurity motion.

3. Askeland Problem 5-38. *Hint: Use the slope of the line.* Using data on diffusion coefficients of different ions in oxides (Figure 5-21 taken from Askeland), calculate the activation energy of diffusion of K ions in β -alumina. Materials such as beta alumina show rapid transport of ions and have been considered for batteries based on sodium and sulfur.

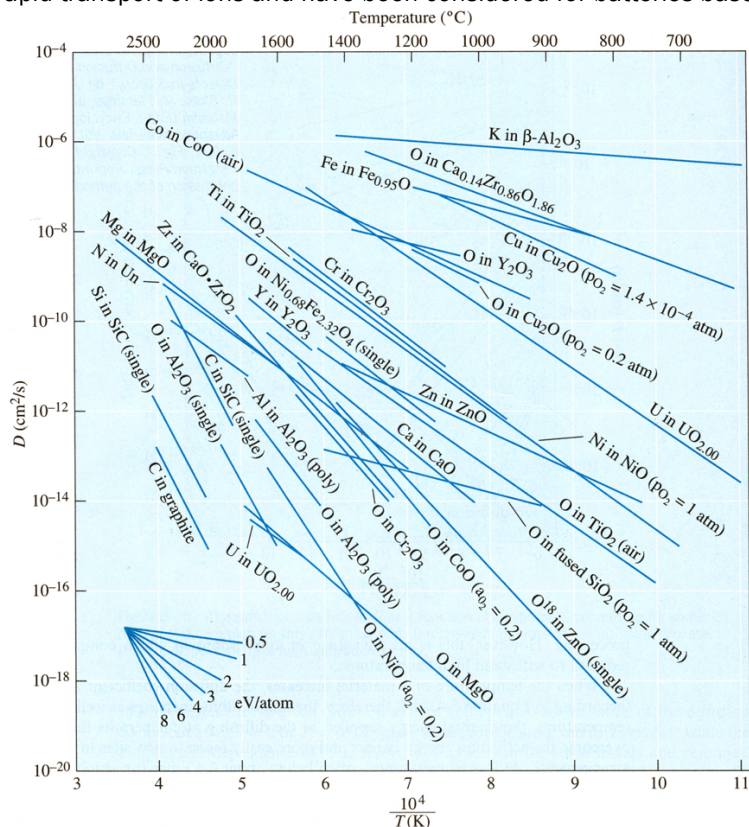


Figure 5-21 Diffusion coefficients of ions in different oxides. (Source: Adapted from Physical Ceramics: Principles for Ceramic Science and Engineering, by Y.M. Chiang, D. Birnie, and W.D. Kingery, Fig. 3-1. Copyright © 1997 John Wiley & Sons. Adapted with permission.)

For this problem, we need to use the equation for diffusivity to calculate the slope of the D vs. 1/T line. Diffusivity is given by

$$D = D_0 \exp\left(\frac{-Q}{RT}\right).$$

Taking the log of both sides of this equation gives

$$\log D = \log D_0 + \left(\frac{-Q}{2.3R}\right)\left(\frac{1}{T}\right).$$

We can see that this looks like the $y=b+mx$ equation for a line with slope m . Thus, the slope of a straight line on a log D versus 1/T curve is given by $(-Q/2.3R)$. Using data for K diffusion in $\beta\text{-Al}_2\text{O}_3$ from Figure 5-21, we have

$$\left(\frac{-Q}{2.3R}\right) = \frac{\log(y_2) - \log(y_1)}{x_2 - x_1} = \frac{\log(D_2) - \log(D_1)}{\frac{1}{T_2} - \frac{1}{T_1}} = \frac{\log(D_2) - \log(D_1)}{\frac{1}{T_2} - \frac{1}{T_1}} = \frac{\log(3E - 7) - \log(1E - 6)}{0.0011 - 0.0007}$$

With these values, Q is about **25,000 J/mole, or about 0.26 eV/atom** – a very small activation energy!