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3.205 Thermodynamics and Kinetics of Materials—Fall 2006

November 2, 2006

Assignment 8: Due Thursday, November 9

1. Figure 1 shows data for the steady-state composition profile of carbon diffusing through a hollow cylinder of iron at $1000°$C.

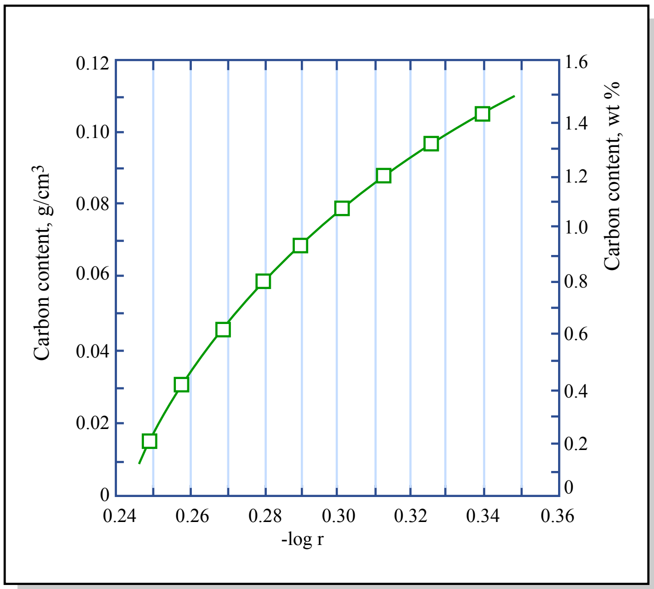

Figure by MIT OCW.

Figure 1: Data for C diffusion in an iron pipe. Steady-state concentration profile for diffusion at $1000°$ C. Units for r are centimeters. Data from R.P. Smith, *Acta Met.* **1**, 578 (1953).

   (a) Find an expression for the steady-state composition profile for diffusion through a pipe of inner radius r_i and outer radius r_o assuming constant diffusivity. The corresponding surface concentrations are maintained at c_i and c_0, respectively.

   (b) Estimate the value of the diffusivity of carbon in iron at $1000°$C using the data in Fig. 1. Do the data support the assumption that the diffusivity is independent of carbon concentration?

2. (Ref: Poirier and Geiger 1994, p. 502.) Silicon is exposed to a gas that establishes a concentration of 10^{18} atoms (Al) per cm^3 on the surface of the silicon. The process is carried out at 1473 K and the diffusivity of Al in Si is 10^{-15} m^2s^{-1} at this temperature.

   (a) After 30 min, at what depth below the surface of the Si will the concentration be 10^{16} atoms (Al) per cm^3?

   (b) Calculate the total amount of Si (in atoms (Al) per cm^2) that has diffused into the Si after 30 min of treatment at 1473 K. The flux at the surface is given by

$$J(x=0,t) = (c_s - c_0)\sqrt{\frac{D}{\pi t}} \tag{1}$$

3. Please solve Exercise 2.6 on p. 108 of Porter and Easterling's text *Phase Transformations in Metals and Alloys.*

4. (Ref: Poirier and Geiger 1994, p. 506.) By ion implantation, lithium can be concentrated in a very thin surface layer (10^{-6} cm) on a nickel substrate. After implanting the surface layer, it has a lithium concentration of 10^{20} atoms cm^{-3}. Determine the time at 1000 K for reducing the surface concentration to 10^{19} atoms cm^{-3}. At 1000 K, the diffusivity of lithium in nickel is 5×10^{-12} $m^2 s^{-1}$.

5. (Ref: Poirier and Geiger 1994, p. 507.) In order to make transformer steel with low losses, a low-silicon iron sheet 2 mm in thickness is to be exposed on both sides to an atmosphere of $SiCl_4$ which dissociates to Si(g) and Cl_2(g). The Si(g) dissolves in the steel up to 3 wt. % Si at equilibrium. Calculate the time necessary for the Si concentration to reach 2.5 wt. % Si at the center of the sheet if the diffusivity is 1.5×10^{-12} $m^2 s^{-1}$ at the processing temperature of 1255 K.

6. A computer simulation of diffusion on a two-dimensional square lattice of screen pixels spaced 0.5 mm apart is carried out. The square simulation cell contains a grid of 101×101 pixels. Initially there is a vacant site at the center of the cell, identical "red" atoms at all other sites, and at $t = 0$ the vacancy begins to execute a random walk of nearest-neighbor exchanges with atoms with a vacancy jump rate of 10,000 s^{-1}.

   (a) Estimate the time it will take the vacancy to reach a site at the edge of the simulation cell.

   (b) Now the simulation is repeated but a single red atom adjacent to the vacancy at the beginning of the simulation is replaced with a "blue" atom. Estimate the time it will take for the blue atom to reach a site at the edge of the simulation cell. Assume that exchanges of the vacancy with red and blue atoms occur at the same rate of 10,000 s^{-1}.