Assignment 9: Due Tuesday, November 21

Note: Problem #1 is held over from Assignment 8. If you already answered it well you do not have to re-submit. If you wish to submit a revised answer you are welcome to do so.

1. 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\(^{-1}\).

2. Please solve exercise 2.9 on page 109 of Porter and Easterling’s *Phase Transformations in Metals and Alloys*.


   (a) Assuming that the particle executes a random walk, what is the relation between \( n \), \( l \), and the mean squared displacement \( \langle R^2 \rangle \)?

   (b) In three totally different experiments it is found that: in one case \( \langle R^2 \rangle = nl^2 \), in a second \( \langle R^2 \rangle = 0 \) though \( n \gg 0 \) and \( l > 0 \), and in a third \( nl^2 < \langle R^2 \rangle < n^2 l^2 \). Explain the different relationships that must exist between the successive jump directions for each of the three cases.

4. (Ref: P.G. Shewmon, *Diffusion in Solids*, Second Edition, p. 220.) As a diffusion expert you are to calculate the thickness of Ag required to maintain at least a 99% Ag alloy on the surface of Cu for 5 years. The most accurate data you can locate is a study of \( D \) for Ag in Cu between 750 and 1050°C. Extrapolating these data to 150°C, you find that a 1 micrometer layer of Ag will last for 150 years. A laboratory test shows that a 1 micrometer silver layer completely dissolves in a sample over a weekend at 150°C. Why might the calculation of the rate at 150°C be invalid?

5. In typical solid-state system, \( \Delta g_B = -2000 \text{ J/mol} \) and \( \gamma = 100 \text{ mJ/m}^2 \). Calculate the critical size \( R_c \) and free energy barrier \( \Delta G_c \) for homogeneous nucleation under these conditions. Assuming that the material is f.c.c. and has a lattice constant of 0.38 nm, how many atoms are there in the critical nucleus? Compare \( \Delta G_c \) to \( 76kT \), assuming a nucleation temperature of 800 K. Is homogeneous nucleation likely under these conditions?