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3.205 Thermodynamics and Kinetics of Materials—Fall 2006

November 14, 2006

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*.

3. (Ref: P.G. Shewmon, *Diffusion in Solids*, Second Edition, p. 129.) A jumping particle of a dilute component in an alloy makes a series of n jumps each of length l.

   (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 $150°$, 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, $\Delta g_B = -2000$ J/mol and $\gamma = 100$ mJ/m^2. Calculate the critical size R_c and free energy barrier $\Delta \mathcal{G}_c$ 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 $\Delta \mathcal{G}_c$ to $76kT$, assuming a nucleation temperature of 800 K. Is homogeneous nucleation likely under these conditions?