Problem Set #3

Due Friday April 29, 2016 at 5 pm

MS133: Kinetic Processes in Materials
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Spring 2016

1. Calculate $\langle \cos\theta \rangle$ and f for a tracer diffusing in a two-dimensional square lattice by a vacancy mechanism. Consider only vacancy exchanges with nearest neighbors, and trajectories which move the solute again in three or fewer vacancy jumps.

2. Consider diffusion of a substitutional impurity in the diamond cubic structure shown in Fig. 3.2. In the presence of a vacancy-impurity interaction there will be four vacancy-atom exchange rates. One, ν_I, is the exchange rate between the vacancy and the impurity. There are three exchange reates which involve an exchange between the vacancy and host atoms: ν_H which is the exchange rate when the exchange does *not* break or form a vacancy-impurity pair, ν_{HB} which is the exchange rate where the exchange *breaks* a vacancy-impurity pair, and ν_{HF} which is the exchange rate where the exchange *forms* a vacancy impurity pair. As usual, consider only nearest-neighbor jumps, and note that there are four nearest neighbors in this structure.

    (a) Given that the vacancy and impurity reside on nearest neighbor sites, what is the probability that the vacancy will exchange with the impurity on the next vacancy jump?

    (b) Considering only vacancy trajectories involving only one jump, calculate the correlation coefficient.

(c) What is the probability that the vacancy will follow the five jump trajectory shown as arrows in Fig. 3.2?

Your answers should be in terms of the four exchange rates.

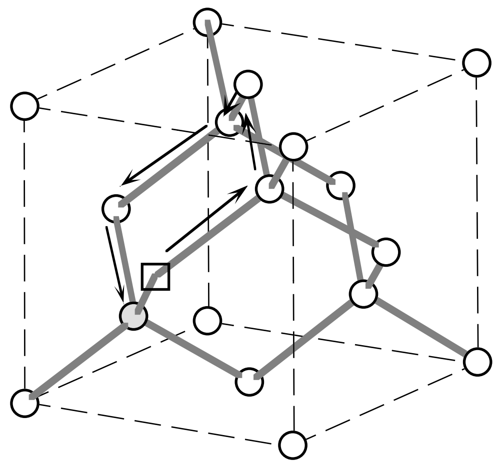

Figure 3.2: Diamond crystal structure showing tetrahedral bond arrangement and grey impurity atom and square vacancy.

3. Consider diffusion of small concentrations of Se in Cu at 1000 K. Use data in the notes and handouts to estimate numerical values answers for the following (again cite any source the numbers you use):

   (a) What is the probability that a Cu atom will have a vacancy as one of its near neighbors. (Consider only free vacancies.)
   (b) Estimate the number of vacancy-impurity pairs for a given atomic fraction of Se.
   (c) What is the probability that a Se atom will have a vacancy as one of its nearest neighbors.

4. In our treatment of diffusion of an interstitial species, for which our prototypical example was C in Fe, we always assumed that the interstitial species was dilute, so that only a small fraction of the interstitial sites were occupied. We now wish to reexamine this mechanism and consider the possibility that an arbitrary fraction x_A of the interstitial sites are occupied, leaving a fraction $x_V = 1 - x_A$ vacant. For simplicity we assume that the interstitial sites form a simple cubic sub-lattice with lattice parameter a_0, and that there is no exchange between the interstitial and host lattice sites.

   (a) In the expression

   $$D = f(sa_0)^2 \nu pjz$$

   evaluate s, p and jz. Describe the process represented by ν.

   (b) Now we turn to calculating the correlation coefficient f. As in the treatment in the text, we examine the situation where an interstitial atom has just jumped to a vacant site. However, now each site around the atom has some probability of being vacant, so a reasonable assumption is that the probability that the atom will jump to a given nearest neighbor site is the probability that it is vacant divided by the number of nearest neighbors. Using this approximation, calculate the correlation coefficient. Examine the cases where $x_V \to 1$ and $x_V \to 0$.