EE539A
Nanotechnology Modeling
Fall 2015

Assignment #4

Due 12/4/15

1. Consider diffusion of O in Si. O is primarily a bond-centered (bc) interstitial. There is a binding energy for adjacent bc interstitial O atoms. The O dimer (pair) is also mobile.

a. Write a set of coupled continuity equations describing the redistribution of O. Identify specific DFT calculations to determine each of the parameters in your equations. Assume that O_i is neutral for all Fermi levels, but that O_{2i} also has 2+ charge states for both the ground and transition states, with the distribution over charge states remaining near equilibrium.

b. If the dimer has a lower migration barrier than the single O_i and charging and pairing reactions are fast, derive an expression for the total oxygen diffusivity as function of oxygen concentration, (n/n_i), and temperature. Sketch qualitatively the expected behavior on an Arrhenius plot.

2. Consider an A/B alloy on an FCC lattice with diffusion via vacancy mechanism. Assume only nearest neighbor interactions with AA, BB, AB, AV and BV interaction energies (assume V concentrations are low so that VV interactions can be ignored). Formulate the free energy of the alloy as a function of composition in a random alloy (no local ordering). Use this energy to derive reaction/diffusion equations as function of NN interactions and A/V and B/V exchange barriers. Describe qualitatively how the system can be expected to behave for different interaction energies and composition regimes.