EE539B
Nanotechnology Modeling
Fall 2015

Assignment #3
Due 11/13/15

1. Use the Metropolis Monte Carlo method to calculate the equilibrium number of step edge atoms (atoms with 5 1st nearest neighbors), step edges (4 1NNs), kinks (3 1NNs), corners (2 1NNs), line end atoms (1 1NN) and adatoms (0 1NN) for a 2D hexagon array of atoms. Consider surface coverages of 0.2 and 0.5 and temperatures of E/k and E/4k, where E is the nearest neighbor (NN) binding energy. You should be able to write a simple program in Matlab or C. Comment on your results.

2. Use KLMC software LAMOCA (see link to manual on course homepage) to simulate interstitial-mediated diffusion of B in Si. Initialize system with B and I distribution and calculate B and I diffusivities at 1000C. Include B/I formation energy of -0.9eV relative to well-separated B and I, and BI and I migration barriers of 0.5eV. Include 1NN BI/I binding of -1.5eV, and 1NN I/I binding of -1.0eV. Compare your results to simple analytic calculations.

3. Use a Monte Carlo method to calculate something of interest to you.

4. Write a paragraph describing your plan for course project.