3.320 Atomistic Modeling of Materials Spring 2003
Problem set 4: Molecular Dynamics

In this problem set, we will look at Ar using molecular dynamics with a Lennard-Jones energy model. First, we will study melting in Ar. Then, we will use molecular dynamics to study annealing in Ar.

Problem 1. Melting temperature of bulk Ar

Find the melting temperature of bulk Ar using molecular dynamics with a Lennard-Jones potential. Some issues to consider are timestep and supercell size. How can you determine if the material is melted? You should come up with as many ways as possible. Make sure to record all of simulation parameters (such as time step, potential and potential parameters, cell size, equilibration time, sampling time, ensemble used, and so on).

Discuss all of your results. Are the results what you expected? How do they compare with experiments?

Problem 2 Ar clusters

The Cambridge cluster database is here.

http://brian.ch.cam.ac.uk/CCD.html

The lowest-energy LJ clusters are listed here

http://www-wales.ch.cam.ac.uk/~jon/structures/LJ/tables.150.html

Build the 38 atom cluster with the minimum energy configuration. Remove (or add) an atom, and use molecular dynamics to anneal this system to find the lowest energy configuration for a 37 (or 39) atom system. How does the energy and configuration you calculate compare with the 37 (or 39) atom configuration listen on the Cambridge cluster database? Make sure to list all of your simulation parameters and to discuss your results.

Problem 3 Short answer

How would you set up a molecular dynamics simulation to find the Pd-V phase diagram? What MD parameters would you need to define? What would be some ballpark numbers you would use? How would you pick these? What system parameters would you need to define? What are some difficulties you would encounter? Is this a good method to simulate phase diagrams? (Figure taken from A.F. Kohan's thesis)