HOMEWORK 6: MOLECULAR DYNAMICS

Due electronically April 11 at midnight

In this homework, you will use the LAMMPS molecular dynamics code package and the OVITO visualization software to explore molecular dynamics simulations. For this assignment, you will need:

- **in.fccVacancy**: LAMMPS input deck for calculating FCC vacancy formation energy.
- **dump.cmu**: Simple LAMMPS dump file of atomic positions.
- **in.2dcrack**: LAMMPS input deck for fracture of a 2D crystal.
- **in.LJexample**: LAMMPS input deck for Leonard-Jonesium, with temperature controlled by a thermostat.
- For general clarification questions, please ask publicly on Piazza. For private questions about the specifics of your code, please email your code to the TA's.

0. (4 pts) Turn in the snapshot of the Σ3 (111) grain boundary from Group Exercise 3-1.

1. Last week, you wrote your own lattice statics code to calculate vacancy formation energy. This week, we use the more advanced capabilities of the LAMMPS code (http://lammps.sandia.gov/) to find a more accurate answer. We run LAMMPS by creating a list of commands/parameters/options in an input deck file. Although one can create input decks entirely from scratch, more often we use a previous input deck as a template. Let's explore an input deck to see how it works.

   (a) (2 pts) The input deck **in.fccVacancy** sets up and runs molecular statics using the Lennard-Jones potential for a perfect FCC crystal and an FCC crystal containing one vacancy. Using the information in the input deck, fill in the system parameters it uses:

parameter	**default value in in.fccVacancy**
number of unit cells per dimension, N_{cell}	
lattice parameter, a_0	
Lennard-Jones ε	
Lennard-Jones σ	
Lennard-Jones cutoff radius r_c	

   (b) (2 pts) Now, use the procedure from Group Exercise 3-1 to run a LAMMPS lattice statics simulation on nanoHUB using **in.fccVacancy** as the input deck. There is a lot of information contained in the standard output file **stdout**, including the information you are looking for: the potential energy U of the perfect and imperfect FCC crystals. Find those data and report them in the table below.

(c) (2 pts) Using your own lattice statics code and the same system parameters, calculate U for the perfect and imperfect crystals and report them in the table below.

Result	LAMMPS	Your code
Potential energy of the perfect FCC crystal, U_{ideal}		
Potential energy of the crystal containing a vacancy, U_{imp}		

(d) (2 pts) If everything has gone well, the potential energy of the perfect crystal is the same in LAMMPS and your code. However, the potential energy of the imperfect crystal will be different by a very small amount. What accounts for that difference?

2. Much of the analysis of an MD simulation involves quantifying the output by analyzing the atomic positions and forces (e.g. identifying defects, measuring local strains, etc.). However, it is also often helpful to look at how the atoms are arranged, that is, visualize the atomic configuration.

(a) (2 pts) Use the OVITO code package to open the included dump file **dump.cmu**. Play around with the viewing options. Some possibilities to explore: Change particle size; turn on/off the boundaries of the simulation cell; rotate, translate, and scale the image; change the color map; add bonds between atoms; anything you like. Attach an image where the atoms are a nice size and color coded by type (as given in the dump file).

(b) (2 pts) Now run a LAMMPS molecular statics simulation of a vacancy in an FCC crystal. Use system parameters from above, except make the number of unit cells per dimension $N_{cell} = 5$ and add a second vacancy, not too close to the first. Report the total potential energy U.

(c) (2 pts) Download and open the dump file for this simulation. Create and attach one image of the system that has all of the following characteristics:
(i) Shows the atoms as spheres of radius 0.56
(ii) Colors the atoms by their energies (as given in the `c_eperatom` column in the dump file)
(iii) Has lines indicating the bounds of the simulation cell
(iv) Includes 2 periodic images in each dimension

3. Of course, the real power of molecular dynamics is the ability to capture dynamics – the time-dependent evolution of the system of atoms. We will use the molecular dynamics capability of LAMMPS to explore rate-dependent behavior during fracture.

(a) (2 pts) The input deck **in.2dcrack** contains an input deck for a 2D simulation of crack growth in a Lennard-Jones crystal. Run the simulation with the default parameters, download the resulting dump file, and view it with OVITO as an animation. Attach snapshots of the initial and final atomic configurations, colored by atom type.

(b) (2 pts) The crack didn't get very far, because you ran it for only a few timesteps. Modify the input deck to run 15000 timesteps, and attach a snapshot of the final configuration.

(c) (2 pts) There is a lot of ancillary damage, because you are pulling the crack open very fast. (Technically, elastic shock waves are interacting constructively to nucleate vacancies, which then grow into voids.) Pull it more slowly (with a rate of 0.05). You will also want to add more timesteps, since things will happen more slowly. Try 42000 timesteps. Attach a snapshot of the final state. Has the ancillary damage decreased?

(d) (2 pts) With the smaller strain rate, the simulation is pretty slow. The code would be more efficient, and perhaps the crack would propagate more easily, if the interatomic potential cutoff distance were decreased. Set $r_c = 1.01$. What happens? Why?

4. One of the most powerful aspects of MD is its ability to capture the effects of temperature, but as we've learned, this isn't as simple as it sounds. In this problem, we will consider an example given in your textbook (section 6.2.2) in order to explore temperature in the NVE ensemble.

   The textbook example is a 6 x 6 x 6 cell periodic FCC crystal of Lennard-Jonesium with $\varepsilon = \sigma = 1$ and a cutoff radius $r_c = 2.5$. All input parameters are in reduced Lennard-Jones units. The initial density (which sets the volume) $\rho^* = 0.55$; temperature $T^* = 0.2$, and time step $\Delta t^* = 0.005$.

   (a) (2 pts) The LAMMPS input deck **in.LJexample** sets up this system. Modify the input deck to include the desired parameters, and attach your modified input deck.

   (b) (2 pts) Now run a LAMMPS molecular dynamics simulation using this input deck. Your textbook goes through considerable effort (using radial distribution functions) to show what is rather obvious when you look at the atoms. Attach a snapshot of the initial and final structure. What has happened to the system?

   (c) (3 pts) Your book presents an excellent discussion of the behavior of the various thermodynamic variables *E, U, K, T*, density, and *P*. Based on what you know about NVE MD, answer the following questions:

      (i) Which thermodynamic variable(s) must be constant in this simulation?

      (ii) Which thermodynamic variable(s) must increase?

      (iii) Which thermodynamic variable(s) must decrease?

      (iv) Which thermodynamic variable(s) must be positive?

      (v) Which thermodynamic variable(s) must be negative?

      (vi) What is the sum of K and U?

   (d) (2 pts) Your simulation has created a file that gives the time evolution of the thermodynamic variables (**LJ-thermo-info.txt**). Make a plot showing the time evolution of *E, U, K, T*, density, and *P*. (There is additional data in this file; do not include it on your plot.) Do the thermodynamic variables behave as you predicted in part (c)?

(e) (2 pts) Finally, as suggested in your book, increase the initial density to $\rho^* = 1.0$ in order to stabilize the solid phase. You will also need to set the initial temperature to $T^* = 1.4$. Attach a snapshot of the final structure. Is the solid phase maintained? Is the final average temperature comparable to that in the previous simulation?