Week 3 – Homework Assignment 3

Molecular dynamics simulations

Problem 1. Simple MD simulation of an Al perfect crystal. Follow the online tutorial on MD simulations of Al melting to setup a MD simulation of bulk aluminum using the nanoMATERIALS simulation tool in nanoHUB.
For this first problem, you will perform a slightly different simulation than the one in the tutorial, a simpler one. Follow the steps in the tutorial except for the changes indicated below:

- Build a supercell by replicating the 4-atom fcc unit cell 5 times along each direction, as shown in the tutorial.
- Use the NVE ensemble (constant energy, volume and number of atoms) as opposed to NPT (constant temperature and pressure) – top of slide 4
- Number of MD steps 5,000 (total simulation time 10 ps)
- Do not increment the temperature (slide 4)

Run the simulation and answer the following questions based on your results.

Question 1.1: Total energy is a constant of motion in Hamiltonian dynamics. Did your numerical experiment conserve energy? Specifically, is the fluctuation in energy considerably smaller than the fluctuations in potential energy?

a) YES

b) NO

This is an important verification step for any MD code. In the NVE ensemble energy should be conserved, otherwise your timestep is too large or the code has a bug. You can try running with a larger timestep and will see the deterioration of energy conservation.

Question 1.2: The instantaneous temperature of the system is computed from the kinetic energy, as we will learn in week 4. The initial value of temperature was 300K in these simulations. How does temperature evolve during the run?

a) The temperature remains rather constant

b) The temperature decreases to a value about half of the original one

c) The temperature increases

We will learn why this happens in week 4.

Problem 2. MD simulation of melting. Now follow the simulation in the tutorial step by step and perform the simulation of melting. After the simulation is done analyze the results and answer the following questions.

Question 2.1. At what temperature do you observe the Al melt? (Melting is indicated by a sharp increase in volume, also take a look at the atomic snapshots.)

a) Approximately at 1,500 K

b) Approximately at 1,000 K

c) Approximately at 2,500 K

Question 2.2. The experimental melting temperature of Al is ~930K. What are possible origins of the discrepancy in the prediction? Select the best answer.

a) The interatomic potential only provides an approximate description of the forces between atoms

b) The system is perfect and the lack of nucleation sites will lead to overheating

c) Both a) and b).

Download the data from the simulation and plot potential energy and total energy (per atom – remember you have 500 atoms in the simulation) as a function of temperature. Fit a straight line to the data for the solid (low temperatures) and estimate the derivative of total energy and potential energy with temperature.

Question 2.3. The derivative of total energy per atom with temperature (specific heat) from the simulation is approximately: (Boltzmann's constant k_B = 0.001987 kcal/mol/K)

a) 30 k_B

b) 0.1 k_B

c) 3 k_B