

Homework #3 (150 points), page 1 of 2

Objective: Building initial system with MSE627-CG code. Understand the connection between the temperature and velocity distribution. Analysis of melting and phase transformations in terms of evolution of kinetic and potential energies.

1. Use MSE627-CG code to create an FCC crystal with $5 \times 5 \times 5$ unit cells (500 atoms). In contrast to homework #2, choose the FCC lattice constant a_{fcc} not from the equilibrium interatomic distance that corresponds to the minimum of the interatomic potential ($a_{\text{fcc}} = 5.4$ Å), but based on the experimental molar volume of liquid Ar at the melting temperature and 1 atm pressure, $29 \text{ cm}^3/\text{mole}$. Give the value of the lattice parameter you use to build the initial system in your report.
2. Find the temperature at which the Ar crystal melts: perform a series of simulations at constant density and different temperatures, so that you have several (3-4) runs below the melting point and several (3-4) above the melting point. Use visual analysis of the final configurations to distinguish between liquid and solid states. Run each simulation for a time sufficient to equilibrate the system and to find equilibrium energies and temperature. Explain your choice of the duration of the simulations. What are the indications that the equilibrium has been reached? What is the temperature after equilibration? To calculate the temperature you should average over a part of the MD trajectory. In your report and analysis use the real temperatures in your system, not the input parameter QTEM.
3. Plot the temperature dependence of the potential energy. Is it possible to determine the temperature of solid-liquid transition from this dependence?
4. For one of the simulations you did in question #2 plot the velocity distributions in the equilibrated system. To get better statistics for the velocity distribution you can accumulate data over a number of timesteps. Compare your velocity distribution with Maxwell-Boltzmann distribution for the same temperature (plot both distributions on the same graph and briefly discuss the agreement/disagreement that you observe).
5. Using MSE627-CG code create BCC **or** Simple Cubic crystal with $6 \times 6 \times 6$ unit cells for BCC **or** $7 \times 7 \times 7$ unit cells for SC. Choose the lattice parameter so that the density of your system is the same as the one of FCC crystal in question #1. Give the value of the lattice parameter in your report. Attach a snapshot of the initial configuration.

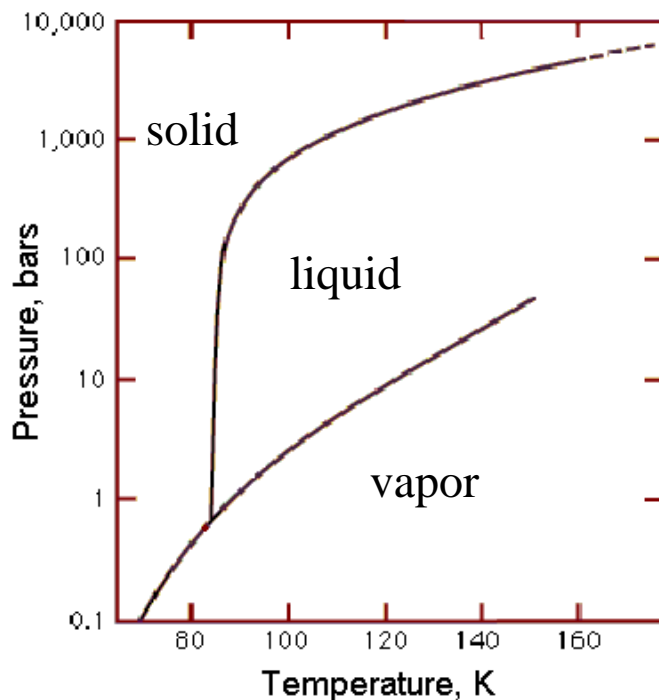
Homework #3, page 2 of 2

6. Perform two MD simulations with periodic boundary conditions for the crystallites that you created in question #5 at $0.5 \times T_m$ and $0.9 \times T_m$, where T_m is the melting temperature of FCC crystal that you found in question #2. Plot snapshots of the final configurations as well as the time dependence of the potential and kinetic energies of the systems. Chose the duration of the simulations so that no significant drift of the potential and kinetic energies is observed by the end of the simulations. **Provide a physical explanation of the time-dependence and values of the potential and kinetic energies.**

7. Repeat one of the simulations described in question #6 with free boundary conditions. Plot snapshots of the final configurations as well as the time dependence of the potential and kinetic energies of the systems. **Provide physical explanation of the time-dependence and values of the potential and kinetic energies. Compare the values of the energies to the ones you obtain in question 6.**

If you have any questions/problems or interesting ideas that you want to discuss – please do not hesitate to send them to the class mailing list.

You can use experimental phase diagram for argon in the discussion of simulation results:



at 1 atm:

$$T_m \approx 84 \text{ K}$$

$$T_b \approx 86 \text{ K}$$

all undergraduate students are getting 20 bonus points for this homework