Homework #4

Objective: Building initial system with MSE627-CG code. Understanding 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 7×7×7 unit cells (1372 atoms). In contrast to homework #3, choose the FCC lattice constant $a_{\text{fcc}}$ not from the equilibrium interatomic distance that corresponds to the minimum of the interatomic potential, but based on the experimental molar volume of solid Ar at the melting temperature and 1 atm pressure, 24.6 cm$^3$/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 at 1 atm pressure: perform a series of simulations at a constant zero pressure and different temperatures, so that you have several (3-4) runs below the melting point and several (3-4) above the melting point. To control pressure, use LFLAG = 1 and IPCON = 1 in md.input. For temperature, do not enforce constant temperature, simply distribute the initial velocities as in homework #3 with KFLAG = 2.

Use visual analysis of the final configurations to distinguish between liquid & 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 may want to average over a part of the MD trajectory after the equilibration. In your report and analysis use the real temperatures in your system, not the input parameter $T_0$. You may want to comment on the reason for difference between the real/final temperature and $T_0$.

3. Plot the temperature dependence of the potential energy (final temperature/energy values after the equilibration, i.e., one point from each simulation). 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 distribution in the equilibrated system. To get better statistics for the velocity distribution you can accumulate data over a number of timesteps (after the equilibration). Compare your velocity distribution with Maxwell-Boltzmann distribution for the same $T$ (plot both distributions on the same graph and briefly discuss the agreement/disagreement that you observe). If you have difficulties with plotting two curves (theoretical and simulated) on the same graph, place two graphs next to each other in your report and use the same scale in both graphs.
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5. Repeat one of the simulations you did in question #2 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. Compare the values of the energies to the ones you obtain in question 2. Provide physical explanation of the time-dependence and values of the potential and kinetic energies.

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:

You can also find more information on the behavior of solid and molten Ar in literature, e.g.,


(you do not need any of this papers to complete the homework – this is extracurricular material)

*all undergraduate students are getting 10 bonus points for this homework*