

H1a MD simulation - static properties

In this homework problem you are asked to use the molecular-dynamics (MD) simulation technique. You will study static properties of aluminum, both in the solid and liquid phase, using an appropriate inter-atomic potential. You should use the units introduced in appendix B in exercise E1, which are units suitable to use in atomic scale simulations.

In the first part, task 1-4, you will develop a basic MD program in C. For your convenience a few C routines are provided. In the second part, task 5-8, you will analyze the output data and determine the heat capacity at constant volume C_V , radial distribution function $g(r)$ and the static structure factor $S(q)$. Here you are asked to develop your own analysis programs.

Task

1. Initiate a system of 256 Al particles on a fcc lattice. Use a suitable lattice spacing. Introduce small random deviations from the initial lattice positions. The displacements should be of the order 5% of the lattice spacing. Solve the equation of motion using the velocity Verlet algorithm and by using periodic boundary conditions. Set the initial velocities to zero and study the time-evolution of the potential, kinetic and total energies. Vary the time step and investigate the effect on energy conservation. What is a suitable time step? (2p)
2. Implement the equilibration routines described in appendix D in the lecture notes "Molecular dynamics". (0p)
3. Equilibrate the system in the solid state, at $T=500^\circ\text{C}$ and ambient pressure. Notice that for these small system sizes used in a simulation study the magnitude of the fluctuations is large. When equilibrating at ambient pressure the instantaneous pressure can become negative. **Hint:** It is useful to study the time-evolution of the simulation cell size for the pressure equilibration.

Determine the temperature T and pressure P using constant energy and volume simulation by making a time-average along the MD trajectory. Convince yourself that the system is in a solid state by plotting the time-dependence of different particle trajectories and verify that the particle trajectories stay close to their initial positions also for long times. (2p)

4. Repeat the previous task for the liquid state, at $T=700^\circ\text{C}$ and ambient pressure. Convince yourself that the system is in a liquid state by plotting the time-dependence of different particle trajectories and verify that the particle trajectories deviate substantially from their initial positions for long times. **Hint:** To melt the system it can

be useful to first increase the temperature above $T=700^\circ\text{C}$ and then decrease it to $T=700^\circ\text{C}$. (2p)

5. The fluctuations of the instantaneous kinetic and potential energies at constant NVE are related to the heat capacity at constant volume C_V for the system. Use the relations in section 7.1.2 in the lecture notes "Molecular dynamics" to determine C_V both for the solid state at $T=500^\circ\text{C}$ and ambient pressure and at the liquid state at $T=700^\circ\text{C}$ and ambient pressure. (1p)
6. Repeat the previous task but now use the relation

$$C_V = \left(\frac{\partial E}{\partial T} \right)_{N,V}$$

from thermodynamics. You should keep the volume V (and particle number N) constant and change the temperature $\pm\Delta T$ with some reasonable value for ΔT . Then evaluate C_V using a finite difference approximation for the above derivative. Compare with the result in the previous task. (2p)

7. Consider now the liquid state system at $T=700^\circ\text{C}$ and ambient pressure. Determine the radial distribution function $g(r)$ (see section 7.3.1 in the lecture notes "Molecular dynamics"). Evaluate also the coordination number $I(r_m)$ by choosing r_m equal to the first minimum of $g(r)$. (3p)
8. Consider again the liquid state system at $T=700^\circ\text{C}$ and ambient pressure. Determine now the static structure factor $S(q)$ by making a direct evaluation of Eq.(55) in the lecture notes "Molecular dynamics". You have to introduce a three dimensional grid in \mathbf{q} -space. The \mathbf{q} -grid has to be consistent with the periodic boundary conditions, *i.e.* $\mathbf{q} = (2\pi/L)(n_x, n_y, n_z)$ where n_x , n_y and n_z are integers. Disregard the delta-function contribution at $\mathbf{q} = 0$. Perform a spherical averaging to obtain $S(q)$.

The static structure factor can also be obtained by integrating the radial distribution function according to Eq.(58) in the lecture notes "Molecular dynamics". Perform that integration and compare your results with the above direct evaluation of $S(q)$. (4p)