

## H1b MD simulation - dynamic properties

In this homework problem you are asked to use the molecular-dynamics (MD) simulation technique. You will study dynamic properties of aluminum, both in the solid and liquid phase, using an appropriate inter-atomic potential.

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 5-7, you will analyze the output data and determine the mean squared displacement  $\Delta_{MSD}(t)$ , the velocity correlation function  $\Phi(t)$  and its spectrum  $\hat{\Phi}(\omega)$ . Here you are asked to develop your own analysis programs.

Use the "Atomic simulation units", introduced in appendix A in exercise E1. You should present your results in a written report. **For instructions how to write the report, read the information on the homepage.**

### Task

1. Fetch and extract the archive `H1.tar.gz` from the course homepage, which contains the code you will use as a starting point. In the `H1main.c` file provided to you, create an array of coordinates representing atomic positions in an fcc lattice using the `init_fcc` function in `H1lattice.c`. The syntax for this is

```
init_fcc(X, N, a0);
```

where `X` is a matrix (in which the atomic positions are stored), `N` is the number of unit cells in each direction and `a0` is the lattice constant. Due to restrictions in the Al-potential, use at least a  $4 \times 4 \times 4$  supercell, i.e. 256 atoms. Create fcc structures of different volume by varying the lattice constant and calculate the potential energy of each generated structure using the `get_energy_AL` function in `H1potential.c`, the syntax of which is

```
E_pot = get_energy_AL(X, N * a0, natoms);
```

where `E_pot` is the variable in which the energy is stored. Write the lattice constant and the corresponding energies to file and determine the equilibrium lattice constant by doing a quadratic fit in Python. Make sure that you can reproduce the data in Fig. 1. What is the theoretical lattice parameter at 0 K? (1p)

2. Introduce small random deviations from the initial lattice positions. The displacements should be uniform in the interval  $\pm 6.5\%$  of the lattice spacing in each direction. Solve the equation of motion using

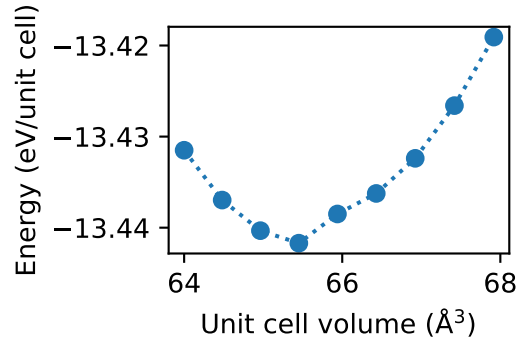


Figure 1: Energy-Volume diagram of aluminium.

the velocity Verlet algorithm, using periodic boundary conditions that are implemented in `alpotential.c`. Set the initial velocities to zero and study the time-evolution of the potential, kinetic and total energies. Compute the average temperature and check that it is around 600-850 K. What is a suitable time step? Vary the time step and investigate the effect on energy conservation. **Hint:** Read section 4.3 in the lecture notes "Molecular dynamics". (3p)

3. Implement the equilibration routines described in appendix E in the lecture notes "Molecular dynamics". Note that the isothermal compressibility can be treated as a constant scaling of the time constant. Further, the isothermal compressibility is the inverse of the bulk modulus. You may use a tabulated value for the isothermal compressibility and the same value can be for both the solid and the liquid state. The time constants should be on the order of at least a few hundred time steps.

Equilibrate the system in the solid state, at  $T=500^\circ\text{C}$  and  $P=1$  bar. Notice that for the small system sizes used in the simulation study, the magnitude of the fluctuations is large. When equilibrating at low pressure the instantaneous pressure can become negative (see Fig. 2). What is the lattice parameter of the equilibrated system? **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 components of the position as a function of time for a few different particles. Verify that the particles stay close to their initial positions also for long times. (4p)

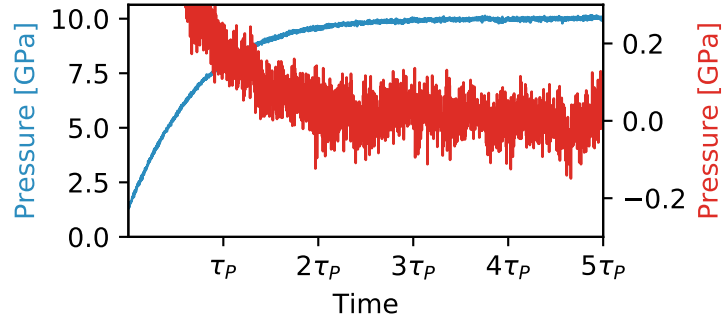


Figure 2: Example of fluctuations during pressure equilibration for high pressure equilibration (10 GPa) and low pressure equilibration (0 GPa).

4. Repeat the previous task for the liquid state, at  $T=700^\circ\text{C}$  and  $P=1$  bar. Convince yourself that the system is in a liquid state by plotting the components of the position as a function of time for a few different particles. Verify that the particle trajectories deviate substantially from their initial positions for long times. What is the lattice parameter of the equilibrated system? **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. Determine the mean squared displacement  $\Delta_{MSD}(t)$ , defined in Eq.(84) in the lecture notes "Molecular dynamics", both in the solid and the liquid state. Use the same temperatures and pressures as in the two previous tasks and for the evaluation of  $\Delta_{MSD}(t)$  use the algorithm described in section 8.1 ("Computational algorithm") in the lecture notes "Molecular dynamics". Determine also the self-diffusion coefficient  $D_s$  in the liquid state (see Eq.(88) in the lecture notes "Molecular dynamics"). (3p)
6. Consider next the velocity correlation function  $\Phi(t)$ , introduced in Eq.(74) in the lecture notes "Molecular dynamics". Use the algorithm described in section 8.1 ("Computational algorithm") in the lecture notes "Molecular dynamics" and evaluate  $\Phi(t)$  both for the solid and liquid state. Perform the integral

$$\hat{\Phi}(\omega) = 2 \int_0^\infty \Phi(t) \cos(\omega t) dt$$

to obtain the corresponding spectrum both for the solid and liquid state. Determine  $D_s$  in the liquid state from the time integral (see Eq.(91) in the lecture notes "Molecular dynamics"). (4p)

7. The correlation function  $\Phi(t)$  can also be obtained by first determine the power spectrum spectrum and then making an inverse Fourier transform using the so called Fast Correlation Algorithm (see appendix G in the lecture notes "Molecular dynamics"). Perform such a calculation to obtain the correlation  $\Phi(t)$ . Compare with the result in the previous task. You should get identical results. (3p)