NB: The graded, first version of the report must be returned if you hand in a second time!

H1b: MD simulation – dynamic properties

Andréas Sundström and Linnea Hesslow

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Task №	Points	Avail. points
Σ		

Introduction

.... TODO... !!!!!!!!!!!!!!!!!!!!

Task 1: potential energy

The theoretical lattice parameter for aluminim can be determined by calculating the minimum potential energy per unit cell in a lattice with zero initial momenta for all particles.

Figure 1 shows the potential energy as a function of the lattice parameter. We used a quadratic fit to find the minimum energy, and obtained $V_{\text{eq}} \approx 65.38\,\text{Å}^3$. This corresponds to the equilibrium lattice parameter $a_{\text{eq}} \approx 4.029\,\text{Å}$ at 0 K, which we took as the initial lattice parameter for the following tasks.

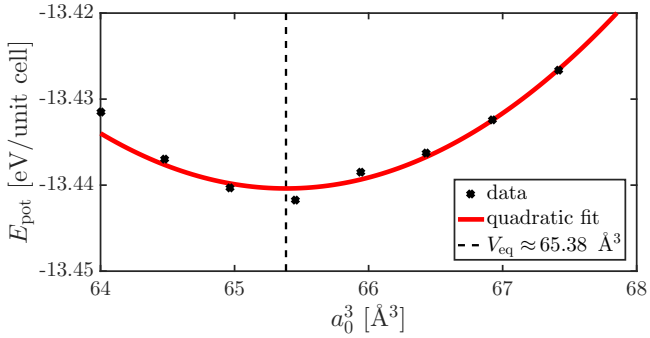

Figure 1: The potential energy per unit cell for aluminum as a function of the lattice parameter cubed.

We find that figure 1 looks similar to the figure 1 in the homework problem file.

Task 2: detmine the timestep

With the random noise, the temperature and the energy are differs between runs, but are in the same order of magnitude. From figure 2, we determine that $dt = 5 \cdot 10^{-3}$ ps = 5 fs is a sufficient time step. This is in line with the lecture notes, where it is stated that the a suitable timestep would normally be a few femtoseconds, or somewhat larger for heavy atoms.

We note that the temperature is higher than desired value of 600-800 K. The temperatures and energies up to one standard deviation are quantified in table 1.

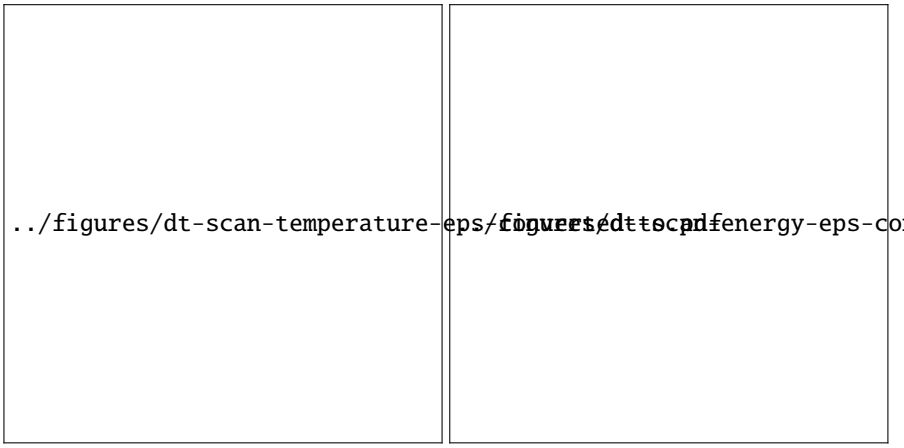

Figure 2: The temperature and kinetic energy per unit cell as a function of time for four different timesteps.

Table 1: Energies and temperatures with one standard deviation uncertainties for four different values of the time steps.

dt [ps]	T [K]	E_{tot} [eV/unit cell]
10^{-2}	$847 \pm 4.2\%$	$-12.55 \pm 1.2 \cdot 10^{-2}\%$
$5 \cdot 10^{-3}$	$1157 \pm 3.8\ \%$	$-12.24 \pm 3.6 \cdot 10^{-3}\%$
$2 \cdot 10^{-3}$	$1058 \pm 3.7\%$	$-12.35 \pm 6.6 \cdot 10^{-4}\%$
$1 \cdot 10^{-3}$	$841 \pm 3.7\%$	$-12.58 \pm 3.6 \cdot 10^{-4}\%$

Tasks 3 and 4: Temperature and pressure equilibration

We set $\tau_P = \tau_T = 100dt$, where $dt = 5 \cdot 10^{-3}$ ps, and equilibrated the temperature and pressure by scaling the particle momenta and positions (and box size) respectively. Choosing a slower equilibration time did not affect the results qualitatively. Both temperature and pressure were equilibrated in the same Verlet loop, but for the higher temperature the the system was first melted by increasing the temperature to 900 °C. To determine the isothermal compressibility κ, the values of Young's modulus Y and shear modulus G were taken from Physics Handbook, table T 1.1. From F 1.15 in Physics Handbook, the bulk modulus can then calculated as

$$B = \frac{YG}{9G - 3Y} \qquad \kappa_{\text{Al}} = \frac{1}{B} \approx 6.6444 \cdot 10^5 \text{ bar}, \tag{1}$$

where $1\,\text{bar} = 6.2415 \cdot 10^{-7}\,\text{eV/Å}^3$ in atomic units. **However, we set $\kappa = 100\kappa_{\text{Al}}$ since the pressure equilibration happened on a much longer timescale than τ_P with $\kappa = \kappa_{\text{Al}}$. We have not yet figured out why this is.**

The results are shown in figure 3, where we overlay the instantaneous values of $\mathcal{T}$ and $\mathcal{P}$ with a moving average using 250 time steps. The desired temperatures and pressures were approximatelyh obtained in the equilibration process. Although the average pressure was slightly below zero, this is within the fluctuation error bars and is in line with the figure 2 in the homework problem document.

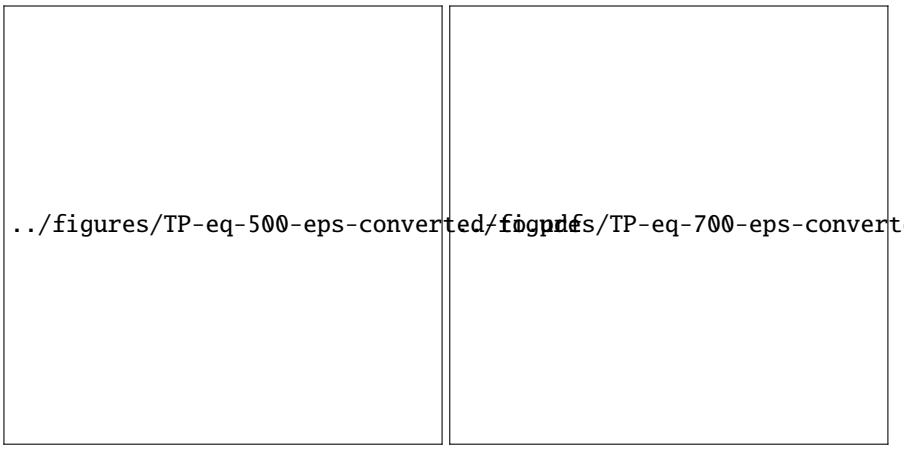

Figure 3: The instantaneous values of $\mathcal{T}$ and $\mathcal{P}$ overlayed with with a moving average using 100 time steps, which corresponds to $\Delta t = \tau_P/2$. Left panel: $T = 500\,°\text{C}$, right panel: $T = 500\,°\text{C}$.

The equilibrium values of the lattice parameter were found to be

$$a_0 \approx 4.10\,\text{Å}, \quad T = 500\,°\text{C}, \tag{2}$$

$$a_0 \approx 4.29\,\text{Å}, \quad T = 700\,°\text{C}. \tag{3}$$

These value are larger than the zero-temperature constants, and it is reasonable that the higher 700 °C case corresponds to a larger lattice parameter at constant pressure.

Tasks 3-5: particle trajectories

Starting with the temperature- and pressure equilibrated systems from the previous section, we study the particle trajectories for both systems. Here, we decrease the timestep to $dt = 5 \cdot 10^{-4}$ ps and the simulation length to $t_{\text{end}} = 5$ ps to get better statistics. This was mostly motivated by increasing the resolution in tasks 6-7.

First, we note that the cumulative averages of the instantaneous temperatures and pressures stayed close to their inital values. This is shown in figure 4.

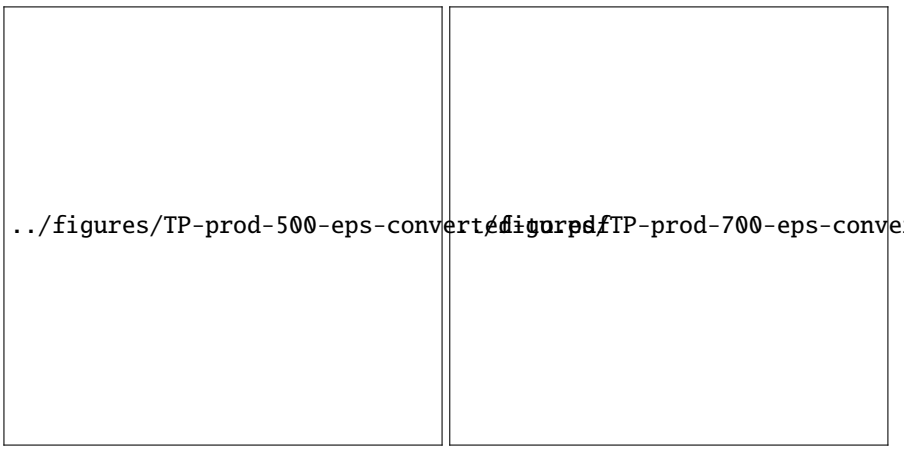

Figure 4: The instantaneous values, and the cumulative averages, of the temperature and the pressure in the production runs. Left panel: $T = 500\,^{\circ}\text{C}$, right panel: $T = 500\,^{\circ}\text{C}$

Task 5

Equation (82) in MD lecture notes:

$$\Delta_{\text{MSD}}(t) = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt' \frac{1}{N_{\text{atoms}}} \sum_{i=0}^{N_{\text{atoms}}-1} \left[\mathbf{r}_i(t+t') - \mathbf{r}_i(t')\right]^2 \tag{4}$$

$$\Rightarrow$$

$$\Delta_{\text{MSD}}(t_k) \approx \frac{1}{N_T - k} \frac{1}{N_{\text{atoms}}} \sum_{j=0}^{N_T-k-1} \sum_{i=0}^{N_{\text{atoms}}-1} \left[\mathbf{r}_i(t_{k+j}) - \mathbf{r}_i(t_j)\right]^2 \tag{5}$$

To determine M, we used mean of ... for t > ...

Task 7

What we did

We calculated the discrete auto-correlation function similarly to the MSD,

$$\Phi_j = \frac{1}{N-j} \sum_{i=0}^{N-j-1} \left\langle v_{i+j} v_i \right\rangle, \tag{6}$$

where $j = 0, 1, \ldots, N-1$ and the average is taken over all atoms. We then preceded to numerically approximate the integral

$$\hat{\Phi}(f) = 2 \int_0^\infty \mathrm{d}t \;\Phi(t) \cos(2\pi f t) \approx 2 \int_0^{T_s} \mathrm{d}t \;\Phi(t) \cos(2\pi f t) \tag{7}$$

using a trapeziodal method in MATLAB, with a frequency range $f = 0$ to $f = 1/(2\Delta t) = f_{\text{Nyqvist}}$, and frequency steps $\Delta f = 1/T_s$, where T_s is a time at about half the simulation

end time. This is to avoid including noisy data in $\Phi(t)$ at later times, where the statistics are poor.

We then calculated the powerspectrum according to

$$\begin{aligned}\hat{P}(\omega) &= \lim_{T\to\infty} \frac{1}{T} \left\langle \left| \int_0^T \mathrm{d}t \; v(t) \mathrm{e}^{\mathrm{i}\omega t} \right|^2 \right\rangle \\ &\approx \frac{1}{T} \left\langle \left| \int_0^T \mathrm{d}t \; v(t) \mathrm{e}^{\mathrm{i}\omega t} \right|^2 \right\rangle \\ \implies \quad \hat{P}_k &= \frac{1}{T} \left\langle \left| \frac{T}{N} \sum_{i=0}^{N-1} v_i \exp\left(\mathrm{i}2\pi \frac{ik}{N} \right) \right|^2 \right\rangle = \frac{T}{N} \left\langle |\hat{\boldsymbol{v}}_k|^2 \right\rangle \end{aligned} \tag{8}$$

where the averages is taken over all atoms, and

$$\hat{\boldsymbol{v}}_k = \sqrt{N} \sum_{i=0}^{N-1} \boldsymbol{v}_i \exp\left(\mathrm{i}2\pi \frac{ik}{N} \right) \tag{9}$$

is the discrete Fourier transform of v_i.

When we compare $\hat{\Phi}_k$ and $\hat{P}_k$ in Figure **??**, we find that they are very similar, as, indeed, they should be acording to the Wiener-Khinthchine theorem.

Concluding discussion

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A Source Code

Include all source code here in the appendix. Keep the code formatting clean, use indentation, and comment your code to make it easy to understand. Also, break lines that are too long. (Keep them under 80 characters!)