Exercise 3 – Computational Materials Engineering

Prof. M. Moseler – WS 2020/2021

Goals:

- Understand the Morse potential for N atoms.
- Understand the concept of periodic boundary conditions (pbc).
- Understand the typical length and energy scales at the atomic scale.
- Understand and learn how to calculate lattice constants.
- Learn how to make pretty plots using matplotlib.

For two particles i and j with positions $\boldsymbol{R_i}$ and $\boldsymbol{R_j}$ (we denote the distance between the particles with $R_{ij} = |\boldsymbol{R_i} - \boldsymbol{R_j}|$) the Morse potential is given by

$$u_2(R_{ij}) = D_0\left[e^{-2\alpha(R_{ij}-R_0)} - 2e^{-\alpha(R_{ij}-R_0)}\right]. \quad (1)$$

As discussed in the lecture, the superposition of pairwise Morse interactions (i.e. every pair of particles interacts via equation (1)) can serve as a simple potential for N atoms

$$U(\boldsymbol{R_1}, \dots, \boldsymbol{R_N}) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N\ \prime} u_M(R_{ij}) \ . \quad (2)$$

D_0, α and R_0 are the parameters discussed in exercise sheet 2.

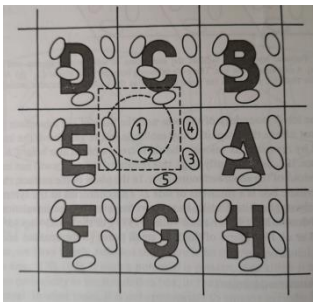
In this exercise we will use such a potential to model copper, silver, lead and nickel crystals.

The typical length scale for atomistic simulations is Ångstrom (Å). 1 Å is one ten-billionth of a metre, i.e. 1 Å = 10^{-10}m. The typical energy scale is electron volt (eV) that was already used during the lecture within the framework of the Bohr model. 1 eV corresponds to approximately 1.6×10^{-19} Joule. All energies and lengths will be measured in multiples of eV and Å throughout this sheet.

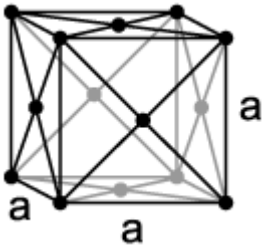
Tasks

Task 1: The crystal structure of the chosen materials is a face-centered-cubic (fcc) crystal. Download and open *"Cu.xyz"* in OVITO to visualize and inspect the copper crystal.

Task 2: We model an infinite copper crystal using periodic boundary conditions, i.e. the system effectively consists of infinite periodic repetitions of the *unit cell* (will be introduced later in the lecture). Visualize some of the periodic images by selecting "*add modification" → "Replicate".*
Remark: To keep the number of interactions finite, each particle only interacts with the closest image of another particle.
For example, in the illustration below, the central box contains 5 particles. Each periodic repetition contains copies of these particles (e.g.1A, 2A… , …4H, 5H). The particle 1 interacts with the closest images of the other particles, which are found in the rectangular box around it (2, 3E, 4E, 5C).
Other interaction schemes (e.g. circular/spherical) may be used to reduce the number of interactions and thus the simulation time.



Task 3: fcc-crystals can be characterized by a single length, the so-called lattice constant a, e.g. the distance between neighboring atoms is $a/\sqrt{2}$, the volume per atom $a^3/4$.



During this exercise we will calculate the lattice constants that minimize the energy for each of the aforementioned materials. For this purpose, we evaluate the energy of the system for different lattice constants (these are the images contained in *"Cu.xyz"*). Download, open and run the file *"lattice_constant.py"*. The parameters for the Morse potential for copper are from the uploaded paper *PhysRev.114.687.pdf*".

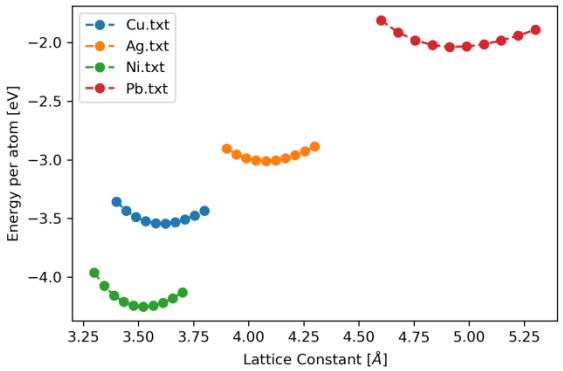
Task 4: Try to understand what the script does. The part where the Morse potential is defined is optional.
How does the size of your structure influence your results? Be careful, the computing effort increases quadratically: $N_{Interactions} = \frac{1}{2} N_{atoms}(N_{atoms} - 1)$. (*ctrl + c* cancels your calculations)
How do the periodic boundary conditions influence the distances in your calculations?
"print()" is a useful function that might be helpful.

Task 5: Compare the lattice constant of copper (that minimizes the energy per atom) that you obtain with the experimental lattice constant listed on Wikipedia (https://en.wikipedia.org/wiki/Lattice_constant).

Task 6: Calculate the lattice constant of silver, lead and nickel using the same method. You can find the parameters for these materials in the lecture slides or in "*PhysRev.114.687.pdf*". Compare to the values listed on Wikipedia.

Task 7: Open "*Cu.txt*" and understand how it is created. Create "*Ag.txt*", "*Ni.txt*" and "*Pb.txt*" for silver, nickel and lead in an analogous way using "*lattice_constant.py*". In each case, the minimum energy and the corresponding lattice constant should be included.

Task 8: Plot the energy per atom as a function of the lattice constant for the different materials in a single diagram. For this purpose, download and run "*plot_energy_vs_lattice_constant.py"*. Try to understand how the script works. Compare the lattice constants of the different materials. The meaning of the different energy values of the materials will be discussed in exercise sheet 4.


Cu.txt
Ag.txt
Ni.txt
Pb.txt
−2.0
−2.5
−3.0
−3.5
−4.0
Energy per atom [eV]
3.25
3.50
3.75
4.00
4.25
4.50
4.75
5.00
5.25
Lattice Constant [Å]