Exercise 4 – Computational Materials Engineering

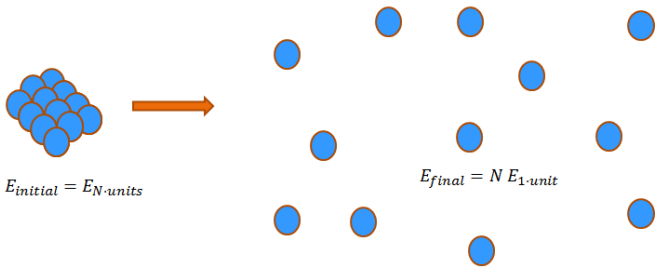
Prof. M. Moseler – WS 2020/2021

Goals:

- Understand and learn how to calculate cohesive energies.
- Understand and learn how to calculate the bulk modulus.
- Learn how to fit functions to a data set using Python.
- Learn how to read and write data with Python.

The potential energy as a function of the lattice constants as calculated in the previous exercise sheet contains, besides the favored lattice constant, other valuable information that will be elaborated on during this exercise sheet.

One of them is the cohesive energy E_c that is a measure for the strength of bonding. It corresponds to the energy needed to transform a condensed matter system into individual units (e.g. molecules, ion pairs or atoms). On this exercise sheet, we define E_c as the energy difference between the completely isolated atoms (i.e. no interactions) and the energy of the crystal, normalized by the number atoms.



$$E_c = \frac{E_{final} - E_{initial}}{N} = \frac{N \times E_{atom} - E_{crystal}}{N} \tag{1}$$

For our interaction via the Morse potential, the energy of an isolated atom is 0. Therefore, E_c is simply given by the energy of the system divided by the number of atoms. Note that this is exactly the quantity that we calculated in exercise sheet 3! In order to get E_c for our materials, we only need to extract the minimum energy of the (lattice constant) – (energy per atom) curves.

The second quantity is the bulk modulus K, a measure of how resistant a material is with respect to compression. Given the energy per atom as a function of the volume per atom $E(V)$, K can be approximated by the curvature in the minimum. More precisely

$$\frac{K}{V_0} \approx \left.\frac{d^2E(V)}{dV^2}\right|_{V=V_0} \tag{2}$$

where V_0 is the volume per atom in the minimum.

The idea behind this exercise sheet is to convert the (lattice constant) – (energy per atom) curves from the previous exercise sheet into (volume per atom) – (energy per atom) curves. Afterwards a parabolic

fit in the minimum of these curves is used to extract the energy in the minimum (i.e. the cohesive energy) and the curvature (i.e. the bulk modulus).

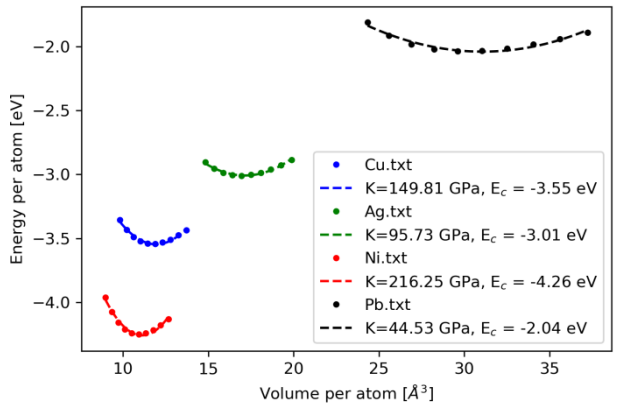
Tasks

Task 1: In order to find the relationship between the lattice constant and the volume per atom, go back to exercise 3 and run the script with "*FaceCenteredCubic(..., size=(1,1,1))*". Open the newly created "*.xyz*" file with OVITO. Your cell should now contain 4 atoms. Study the dimensions of the cell (by clicking on "*Simulation Cell*"). What is the relation between these dimensions and the lattice constant? What is the volume of the cell? How can you calculate the volume per atom based this volume?

Note: The energies that you calculate with this small cell are nonsense. Why?

Task 2: Download "*bulk_modulus.py*" from ILIAS and save it in a newly created folder. Copy the "*Ag.txt*", "*Ni.txt*", "*Cu.txt*" and "*Ni.txt*" files from the previous exercise into the same folder. Make sure that you created them with "*FaceCenteredCubic(..., size=(7,7,7))*".

Task 3: Run the script and try to understand what it does. The resulting plot should look similar to the one below.



Task 4: For each of the curves a parabolic fit with the functional form $f(x) = ax^2 + bx + c$ is performed. As apparent from the script, V_0 (see equation (2)) is calculated by $V_0 = -\frac{b}{2a}$. Derive this formula.

Task 5: Afterwards, K is calculated via $= 2 \cdot a \cdot V_0$. Where is the factor 2 coming from? Note that the script converts the unit of the bulk modulus from $\frac{\text{eV}}{\text{Å}^3}$ to GPa.

Task 6: Why is the cohesive energy calculated as $E_c = -\frac{b^2}{4a} + c$?

Task 7: Compare the cohesive energies you obtain with the cohesive energies listed on http://www.knowledgedoor.com/2/elements_handbook/cohesive_energy.html

Task 8: Compare the bulk moduli you obtain with the information listed on https://en.wikipedia.org/wiki/Elastic_properties_of_the_elements_(data_page)