

HOMEWORK 10**Due: 4:00 pm, Monday, March 6****Problem 1: Calculation of lattice constants and energies**

In this problem, we look at relaxation and total energies. In experiments, a crystal structure in equilibrium is automatically at its correct lattice parameter, which is also the lowest energy configuration. In calculations, we know neither the equilibrium lattice parameter nor the lowest energy configuration beforehand. In calculations, we pick an initial configuration (unit cell, atom positions), and then find the equilibrium (lowest energy) configuration. This is called “relaxation”. There are two types of relaxations. The first type is unit cell relaxations; the second type is atomic positions relaxations. To find the lowest energy geometry, both unit cell and atomic positions must be fully “relaxed”.

A. Calculate the lattice constant and total energy (in eV) for FCC Au. This calculation will be done with the supplied Lennard-Jones potential (input file `gulp1a.in`). Determine the result in two different ways:

1) By using the minimizer in GULP, which performs relaxations automatically. Make sure the `opti` flag is set in the first line of the `gulp` file.

2) By plotting the energy for a few lattice parameters near the equilibrium lattice parameter. Edit the `gulp` input file so that `opti` is replaced by `single`. Then, you will need to manually edit the unit cell parameters in the `gulp` input file (after the keyword ‘`cell`’).

B. Repeat this calculation using the supplied EAM potential (input file `gulp1b.in`).

C. How do the EAM and LJ lattice constants compare with experiments (the experimental lattice parameter for Au is 4.08? Is this expected? Why or why not? The energies for the two calculations (1a and 1b) will be different. Comment on this.

Problem 2: Material structure determination

In this problem, we will compute the structure (HCP or FCC) of a set of materials. Find the difference in energies between the FCC and HCP structures for the two metals, Copper and Aluminum. The structure with the lower energy is the more stable one. Compute the total energies using both a Lennard-Jones and an EAM potential. Note that we are interested in the difference in energies and not the energies themselves.

The needed parameters for the LJ potential are given here for your convenience:
(a) for Al, $A=170605.9$, $B=518.696$; (b) for Cu, $A=44178.11$, $B=267.792$.

Problem 3: Calculation of the vacancy formation energy in FCC Au

In this problem, we will look at many of the issues involved in total-energy calculations. We will look at supercell convergence, effect of relaxations, and shortcomings of potentials. The vacancy formation energy of a crystal, $E_{f,vacancy}$ is given by the cost of removing an atom and putting it in the bulk.

$$E_{f,vacancy} = E_{cell\ with\ (n-1)\ atoms\ on\ n\ sites} - \frac{n-1}{n} E_{perfect}$$

where n is the number of sites in the supercell

A. Compute the vacancy formation energy for Au using the Lennard-Jones potential provided. Compute the vacancy formation energy as a function of different supercell sizes (you can pick which ones). Use the supercell construction available in Gulp. Do not relax your cell after you take out the atom (make sure single, not opti, is at the top of your gulp input file). What is the ratio of the vacancy formation energy to the cohesive energy? Is this what you would expect?

B. Repeat these calculations, but this time relax the cell after removing the vacancy (make sure opti, not single, is set in your gulp input file). How does the vacancy formation energy change compared with non-relaxed calculations?

C. Compute the vacancy formation energy using the EAM potentials provided. Do it as accurately as you can. Use what you learned in parts A and B. You can do it any way you like, but show work.

D. How do the “final” answers from part A and part B compare? The experimental vacancy formation energy for Au is 0.9 eV. Comment on your results, in light of the agreement in problem 1.

Problem 4: Calculation of surface energy

A. Compute the surface energy of a solid (100) surface of FCC Au using the LJ potential. How you do this is up to you, but remember the issues of supercell size and relaxations. In your answer, make sure to write down the formula you use. Give your answer in eV/Angstroms².

B. Compute the surface energy of a solid (100) surface of FCC Au using the EAM potential. In the interests of time, you can skip relaxations.

Problem 5: Calculation of elastic constants

A. For FCC Au, calculate C_{11} , C_{12} , and C_{44} using the given LJ Potential. To do this, you will need to compute the energetics of deformation, and fit the resulting energy curves.

B. For FCC Au, calculate C_{11} , C_{12} using the EAM method. To do this, you will need to compute the energetics of deformation, and fit the resulting energy curves.