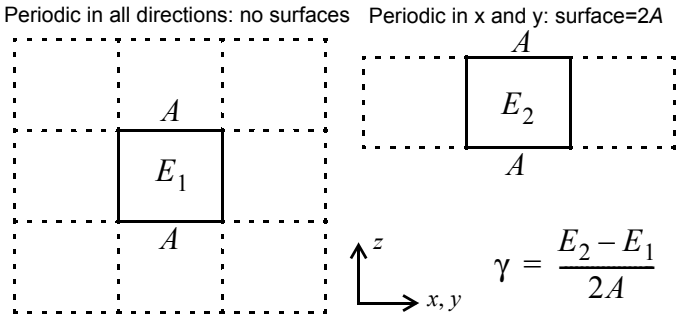
Molecular dynamics 2015

Exercises 10 (not to any specific chapter): `mdmorse` : surface and defect energies

1. (10 p) Surface energies of Cu.



Determine the surface energies γ of our Morse copper at 0 K for the (001) and (111) surfaces[1]. Surface energy can easily be calculated by comparing a simulation with periodic boundary conditions in all directions with one having e.g. z direction open.

Use system sizes of $5 \times 5 \times 5$ unit cells for the (001) surface and $7 \times 4 \times 4$ for the (111) surface. Give the result in units of J/m^2.

Compare the energies you obtained to experimental and *ab initio* results found in article[2]: Q Jiang, H M Lu and M Zhao, *J. Phys.: Condens. Matter* **16** (2004) 521-530.

What happens to the outermost atomic layers? What would happen if atoms only interacted with their nearest neighbors?

Plot the potential energy of atomic layers as a function of z (or distance from the surface). Do the systems seem to be large enough to be used in this kind of calculations? Check your result for (001) surface by doubling the system size[3] and calculating the surface energy for it.

Can you explain the possible difference or equality of the energies of the two surfaces?

2. (5 p) Vacancy formation energy of Cu.

Determine the vacancy formation energy of copper. How does it compare with the cohesion energy? Calculate how large is the effect of relaxation of atoms around the vacancy.

3. (5 p) FCC vs. HCP

a) How large must the pair potential cut-off radius be (in units of nearest-neighbor distance) in order to get differences in potential energy between the FCC and HCP lattices?
b) When only the nearest neighbors are included in energy calculation do the energies of the two lattices differ when the potential energy model is (i) EAM or (ii) a model with explicit angular dependence (i.e. has bond-angle dependence)?

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1. To build the (111) system use the program of exercise 1.
2. The journal is available on-line from University computers at http://www.iop.org/EJ/abstract/0953-8984/16/4/001 .
3. In which direction(s)? Decide yourself.