Please read this compendium before the lab session.

Practical Lab Session in Computational Physics:
TFYA92

Molecular dynamics simulations II

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Lab session II

Upon completion of your login, please follow the instructions given in the first MD lab session to launch MDSinecura. From the Main window choose the same Workplace as last time.

Exercise 1.

Start a new project called ***metal***. In the new project, start a new simulation using the LJ potential, and choose the following metals to work on, paying attention to the PC number on which you are logged in:

- PCs 0 & 1: Cu (name simulation ***LJ_copper***)
- PCs 2 & 3: Ni (name simulation ***LJ_nickel***)
- PCs 4 & 5: Ag (name simulation ***LJ_silver***)
- PCs 6 & 7: Pt (name simulation ***LJ_platinum***)
- PCs 8 & 9: Al (name simulation ***LJ_aluminum***)

Use the indications received in Exercise 1 (previous lab session) to set up and run a 20000 time steps MD simulation at 300 K, 15 cells in each Cartesian coordinate, etc, with a thermostat of your choice. You should also allow for MDSinecura to calculate the specific heat (C_V), mean square displacement (MSD) and radial distribution function (RDF). Make sure you allow for proper relaxation time for equilibrium to be reached before you start these calculations (you have this option under the CALCULATIONS tab).

Upon completion of the MD simulation, calculate for the respective metal the diffusion constant, Lindemann constant and Debye temperature. As in the last lab session, write down the values obtained, your comments and observations.

Exercise 2.

Find the ideal lattice constant for the metal you are working with, using the Lennard-Jones potential. Use the procedure you applied for Argon last lab session to set-up six (6) new simulations, in which you increase the lattice constant value in increments of 1% (positive and negative), starting from the value listed under the POTENTIAL tab. Sketch a graph of energy vs. distance to determine the ideal lattice constant.

Exercise 3.

Start a new simulation, however, this time using the Embedded Atom Method (EAM) potential for the metal you're working with. You should name the simulation, as for the LJ simulations in Exercise 1, ***eam_metal*** (metal = Cu/Ni/Ag/Pt/Al). Use identical parameters as for the LJ simulation in Exercise 1 (number of atoms, time steps, temperature, thermostat, etc), to calculate the same properties, in the same manner. Compare your results with those obtained using the LJ potential for the respective metal.

Exercise 4.

Find the ideal lattice constant, for the metal you're simulating, this time using the EAM potential. Compare your results with the lattice constant value obtained using the LJ potential.

Exercise 5.

Start a new simulation which you can name ***meam***. Clearly, this means that you'll be using the Modified Embedded Atom Method potential. Students already working on Al, Cu and Pt should choose the same metal under GEOMETRY. All other students should choose Ti for the MEAM potential simulation, also under GEOMETRY (please note that Ti is an hcp, meaning total number of atoms will change if you choose 10x10x10 unit cells in X, Y and Z). Use the same parameters as before, except the NUMBER of TIME STEPS which should be set at **10000**, to calculate the same properties as before. Run the MEAM simulation, write down the results, and compare with the corresponding values for the LJ and EAM simulations (valid only for students working on Al, Cu and Pt). Students working on Ti, compare the obtained values with the tabulated values at the end of the lab notes.

Exercise 6: (001) surface energy formation

The surface energy is the energy difference between a system with a surface and an ideal bulk system. The commonly used unit is $eV/Å^2$. The surface energy is normally positive, since it costs energy to create surface, a process which involves breaking interatomic bonds.

Copy the configuration obtained from the EAM bulk simulation (Exercise 3) to a New Simulation which you should call ***surface_001*** (remember to open the Visualization in the EAM simulation, move cursor to the **last step** in the movie, then right-click on the Visualization tab and choose New Simulation From Current Time Step). The easiest way to create a 001 surface at this point is to simply remove the periodic boundary conditions in the Z-direction (you have this option in the CONFIG/*Simulation* window). Make sure you allow for ***free space*** in the Z-direction equal, or close to, the lattice constant value for the respective metal. Run the EAM surface simulation (make sure you allow for Visualization), write down the value of the potential energy, and compare with the value calculated in EAM bulk simulation (obviously, for the metal you're working with).

Questions:

a) What is the surface energy (in $eV/Å^2$)? *Hint:* The area of the unit cell can be calculated from the GEOMETRY window. How much surface area have you created by removing the periodic boundary conditions in the Z-direction?

b) In the starting configuration of the simulation, the atoms should be slightly displaced from their ideal lattice positions. Why? As the surface simulation proceeds, note that some atoms will move further away from the starting bulk positions. Which atoms are these? What is happening? Why?

Exercise 7: Adatom adsorption energy on the (001) surface

Copy, as in the previous exercise, the last step configuration obtained in the ***surface_001*** simulation, to a new simulation called ***adatom_001***. Add a metal atom on the surface (use the Surface tab in the GEOMETRY window). This single atom on the surface is called an adatom. Note that it is possible to adjust the starting position of the adatom. Where should the adatom be placed on the surface to continue the fcc stacking sequence? At what distance? Run the simulation (with visualization) and compare the potential energy with the one obtained in the previous exercise.

Questions:

a) What is the adatom adsorption energy? Hint: The adsorption energy is the energy gained when an atom binds to the surface.

b) Does the adatom move from the position where you placed it? What is the most stable position?

Exercise 8: Dimer adsorption energy on the (001) surface

The dimer (two adjacent, bonded atoms on the surface) represents the smallest possible island. Copy the last step of the simulation obtained in the previous exercise to a new simulation called ***dimer_001***. Form a dimer by placing another surface adatom next to the first one. Where should the second atom be placed on the surface, to properly continue the fcc layering? Run the simulation (with visualization) and compare the potential energy with the one obtained in the previous exercise.

Questions:

a) What is the dimer adsorption energy? Compare the value (per atom) to that obtained for adsorption of an adatom.

b) What does this tell you with respect to thin film growth on this surface?

Exercise 9: Bulk (111)

Create a new simulation for these calculations, and name it ***bulk_111***. You can/should delete some of the previous simulations, since you might run into memory/disk space problems. Use the same simulation settings as for the previous calculations (number of time steps, temperature, thermostat, etc). To create the (111) atomic slab, press the GEOMETRY/Surface Bulk tab. Therein, choose the appropriate Miller indices (111 in this case). Create a 9 layers (111) slab (use the Green '+' and/or '-' cursors in the lower part of the tab) with layer type common, with 16x18 periods in the x-, respectively y-directions. This should create an atomic slab containing close 5200 atoms (note the exact number when you run the simulation). Run the simulation (with visualization) and write down the total potential energy value.

Exercise 10: (111) surface energy formation

Copy the simulation in the last exercise to a new simulation and name it ***surface_111***. Use the same simulation settings as for the previous calculation (number of time steps, temperature, thermostat), but change to NO periodic boundary conditions in the Z-direction with appropriate free space in Z. Run the simulation (with visualization) and write down the total potential energy value.

Questions:

a) What is the energy formation of the (111) surface? Hint: the area of the surface can be calculated using the GEOMETRY/Layer Group. Here you will find the length for each period in the x- and y-directions.

b) Compare this value of the surface energy to the one obtained for the (001) surface. Which surface should be most commonly occurring in nature?

Exercise 11: Adatom and dimer adsorption energies on the (111) surface

Use the procedures described for the (001) surface and add an adatom on the (111) surface. Try firstly the position corresponding to the bulk (fcc) stacking sequence (…ABCABC…), then the position suggested by MDSinecura, which corresponds to the "wrong" (hcp) stacking sequence (…ABABAB…). You can name the two simulations ***adatom_fcc_111***, respectively ***adatom_hcp_111***. Write down and compare the adsorption energies in each case.

Upon completion of the two simulations above, add two atoms in fcc positions to form a dimer on the (111) surface. Call the new simulation ***dimer_111***, run the simulation and calculate the dimer adsorption energy.

Questions:

a) What are the adatom adsorption energies in the two different positions? Which of the two adatom positions, fcc or hcp, should be more stable? Does your result confirm this fact?

b) What is the dimer adsorption energy on this surface? Compare this value with the adsorption energy for the single adatom in the fcc position.

c) Compare these values with those obtained for the 001 surface.

Exercise 12: Trimer adsorption energy on the (111) surface

Place a third adatom in a fcc position on the (111) surface containing the dimer to form a "triangle". This island is called a trimer, so name the simulation ***trimer_111***. Run the simulation, write down the relevant quantities.

Questions:

a) Calculate the trimer adsorption energy and compare the result (per atom) with the values obtained for adatoms and dimers.

b) What does this tell you with respect to thin film growth on this surface?

Exercise 13: Irradiation with energetic species

Add ONE 10 eV bombarding atom to any of your ***surface_simulations*** (you can also use any of the simulations with dimers or trimers). Use the Atom Bombard tab in the GEOMETRY window. Set the x, y values for the start and target points so that the bombarding atom hits the surface/cluster at a moderate angle, say 45 degrees. Run the simulation with visualization.

Questions:

a) What is the effect of the bombarding atom? What impact could this process have on thin film growth? How are the energetic/irradiating atoms created in real life experiments?

If you have time left:

Experiment with bombarding at different energies and/or incidence angles. What happens at higher/lower energies? Do you see any effect based on the angle of impact? How can these processes be related to film growth?

Molecular Dynamics lab survey questionnaire

In order to improve the quality of the lab sessions in the course, please answer the following questions. Just circle what you think is appropriate and place it in my mail box, or give it to me when we meet at the next lecture (in some cases you can circle more than one option). Student identity is naturally not required, you should remain anonymous.

1. How did you find the lab sessions:
   a) boring b) interesting c) enjoyable d) strenuous e) confusing

2. Do you think the amount of work is:
   a) too high b) too low c) appropriate

3. Were the lab exercises:
   a) too easy b) too difficult c) appropriate complexity

4. What do you think of lab exercises, are they useful for learning MD:
   a) yes b) no c) not really

5. Do you find lab exercises connect with the material given in lectures:
   a) yes b) no c) somewhat

6. In case you answered YES at question nr. **5** above, how much does this help:
   a) not at all b) a little c) considerably d) much e) very much

7. Do you think the lab settings correspond to the requirements of a computational course:
   a) not at all b) a little c) somewhat d) pretty much e) very much

8. How did you find the lab compendium:
   a) not at all useful b) somewhat useful c) useful d) very useful

9. What about my own efforts, do you think I was able to devote enough time to your needs:
   a) not at all b) barely enough c) just enough d) sufficient e) plenty

10. If you have any suggestion for how to improve the MD lab sessions, please state here briefly.

Thank you for your cooperation and help!