Materials Physics & Design I: Hands-on Exercises

Molecular Dynamics: Dislocation Motion in Silicon

Forword

In this Hands-on Exercise, you will simulate the ground state and the motion of screw and edge dislocation in silicon (cubic diamond structure). We aim at illustrating and understanding

- How atomistic data are structured?
- How atomistic simulations are performed?
- How the outcomes of the simulations look like?
- What a dislocation looks like at the atomic scale?
- How does a dislocation *really* move?
- …

Start-up

Login to MS Windows with the following credentials:
User: `XXXXXX`
Password: `XXXXXX`

Download the files from the provided location.
Copy this folder under your desktop. This will be your *Working Directory.*

Do not work directly in this folder: it is shared with all class members

Browse with the *Explorer* the content your just copied working directory:

- **`npp.7.5.9`**
  Powerful text editor. Lunch it with `notepad++.exe`. https://notepad-plus-plus.org/.
- **`ovito-2.9.0`**
  Scientific visualization and analysis software for atomistic simulation data. Lunch it with `ovito.exe`. Documentation in http://ovito.org/.
- **`simulations`**
  directory that contains the simulation parameters and from where you will run the simulations (within the *Command Prompt*).
- **`configurations`**
  contains atomistic configurations.

Using the command prompt of MS Windows

Now, browse with the *Command Prompt* the content this directory by following these instructions:

1. To lunch the *Command Prompt,* in the search bar, near the Windows Start Menu, type `cmd` and open the desktop-app called *Command Prompt* (*Eingabeaufforderung*).
2. The *Command Prompt* is a window containing grey text on a black background. The text indicates your *current directory*, and the blinking cursor indicate that it is waiting for you to enter a *command*. It allows you the control MS Windows by entering a commands with the keyboard. You type a *command* followed by one or several *arguments*, and validate by pressing the Enter key. The results of your *command* is then displayed in the

Command Prompt. When the action initiated by your *command* is finished, the cursor blink again and you can enter another *command*.

3. Here is a short list of commands:
   - `dir` display the content of the current directory (no argument)
     example: `dir`
   - `cd` move into the directory specified as argument
     example: `cd Documents`
   - `cd ..` move back into the previous directory (the argument is "`..`")
     example: `cd ..`
   - `d:` switch to the drive called d
     example: `j:`
   - `more` display the content of the text file directly inside the *Prompt*
     example: `more readme.txt`
     If the file is longer than the *Prompt*, you scroll down by pressing `Enter` or `Space`. You can quit the file before the end by pressing `q` .
   - More information can be found online:
     https://www.computerhope.com/issues/chusedos.htm
4. Browse the directories, understand the information given by the command `dir` and try to open some text files with the *command* `more` (for example, files that are in the folders *configuration* or *ovito*).

Important Note:
Space between characters is VERY important while using the Command Prompt.
"Autocomplete" an argument (eg. name of a directory) by pressing the key tab.
Interrupt any command (too long, stucked,…) by pressing ctrl+c .
To copy-paste with the mouse within the Prompt: select the text with the left button, then double-click with the right button.

Atomistic configurations: bulk silicon

Here, we will look at the atomistic configuration (directory `configurations`) that will use in our MD simulation.

1. Lunch Notepad++, then `File > Open` and select the atomistic configuration.
   - Identify the header (first lines) from the core (other lines) of the file.
   - What information are the header?
   - What information are in the core? In Details?
   - How many lines are in the file?
   - How many atoms are represented in this file?
   - What are the dimensions of the simulation box?
2. Close Notepad++
3. Lunch *Ovito*, then `File > Load File` and select the atomistic configuration
   - What represents the 4 sub-screens? How do you change the *View Type* in each of them?
   - Rotate the structure (left click + drag). Zoom in and out (scroll). Span the structure (middle click + drag).
   - Suggest an explanation for the colour of the axis? In which axis the sample is the smallest? Why is it interesting to have such a small direction for the simulation of a single infinite straight dislocation?
   - What are the differences between the files? What do represent the digits in the filename?
   - Note the *Add modification* menu on the right. Select the modifier "Identify diamond structure". What do you see? What do the colour represent?

Motion of a screw dislocation in silicon

Here, we will simulate a screw dislocation in silicon. Especially, we will look at the structure of the dislocation core and simulate its motion.

1. Go in the directory `simulation_screw`
2. Look at the 2 configurations with *Ovito.* What do you see? What is the difference? To help you to see something, you can use the modifiers: Identify diamond structure OR Displacement vector (with the bulk configuration as reference) + color coding
3. Look at the file `relax.lammps` with Notepad++. It is a list of parameter used by the program LAMMPS (https://lammps.sandia.gov/) to perform a simulation.
    a. Try to guess what do they mean.
    b. Note the very first line.
    c. What is doing the line with "boundary…"?
    d. What is doing the line with "dump…"?
    e. What is doing the line with "fix freez…."?
    f. Online documentation : https://lammps.sandia.gov/doc/Commands_all.html
    g. Maybe running the simulation will help you (next step)
4. Simulate the relaxed state of the dislocation
    a. With the Command Prompt, ensure to be in the directory: `\simulation_screw\` of your working directory
    b. Execute the command: `lmp_serial -i relax.lammps`
    c. Wait for the end of the simulation
    d. With Ovito, open the file ending with ".atom". What do you see?
5. Simulation the motion
    a. With Notepad++, look at the file `md1.lammps` and `md2.lammps`. What are the differences? How do they compare with `relax.lammps`?
    b. Replace the "XXXXXX" with the correct parameter. You can help you by looking at the file `relax.lammps`. Think that you want now to perform a simulation by using the relaxed state of the dislocation, that is the RESULT of the previous simulation…
    c. As above, run **successively** the simulations `md1.lammps` and `md2.lammps`.
    d. What are the differences? Why this differences? Which simulation is leading to a moving dislocation?
    e. ***Bonus:*** from the file `log.lammps` (with Notepad++), note the evolution of time during the simulation. By combining this information with the position of the dislocation shown within Ovito, what is the approximate velocity of the dislocation?
    f. ***Bonus:*** from the file `log.lammps` (with Notepad++), note the stress that acting on the dislocation. What is its initial value? How does it evolve? *(Note that this is NOT the Peierls stress)*

Motion of an edge dislocation in silicon

Here, we will simulate an edge dislocation in silicon. Especially, we will look at the structure of the dislocation core and simulate its motion.

1. Go in the directory `simulation_edge`
2. Note the 2 configurations that both contain and edge dislocation: `edge_Si_x-110y111z11-2.lmp` and `edge2_Si_x-110y111z11-2.lmp`. What is the difference?
3. As for the screw dislocation, look at the parameters files that end by ".lammps".
4. Compare relax1.lammps and relax2.lammps?
5. Simulation successively the relaxed state of "edge" and "edge2" with "relax1" and "relax2" (4 simulations in total).

6. Compare the results. What are the differences?
7. Use the result's file `relax2_edge2_Si_x-110y111z11-2.lmp` to run the simulation with the parameters from `md1.lammps`. Is the dislocation moving?
8. Use the result's file `relax2_edge2_Si_x-110y111z11-2.lmp` to run the simulation with the parameters from `md2.lammps`. Is the dislocation moving?
9. ***Bonus:*** from the file `log.lammps` (with Notepad++), note the evolution of time during the simulation. By combining this information with the position of the dislocation shown within Ovito, what is the approximate velocity of the dislocation?
10. ***Bonus:*** from the file `log.lammps` (with Notepad++), note the stress that acting on the dislocation. What is its initial value? How does it evolve? *(Note that this is NOT the Peierls stress)*