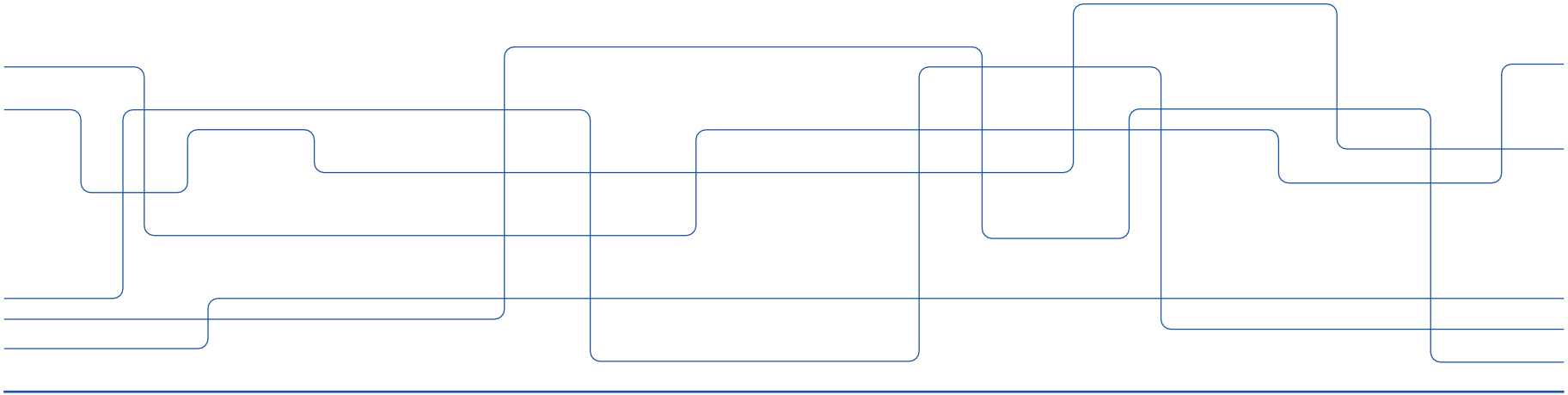
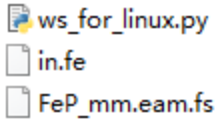
Instruction of using LAMMPS to calculate threshold energy

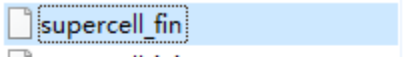




1. Firstly, we have a folder containing the directory of 3 typical lattice directions.
2. Enter one of them, here we take 111 direction as a example.
3. You will see 3 files, the potential file, the input file (in.fe) and the python script which will analyze the results.

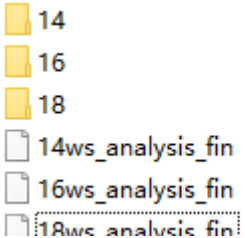
4. Execute the command

```
nohup mpirun -np 4 /home/qigui/lammps/lammps-22Aug18/src/lmp_mpi -in in.fe >/dev/null &
```



5.After some time, you will see folders containing simulation results (14, 16, 18…). The numbers mean the initial PKA energy in eV.

6.Inside each folder, there are two files, the “supercell_fin” is the simulation results. The “ini” is the reference cell.




```
# number va inter
0 0 0
1 0 0
2 0 0
3 0 0
4 0 0
5 0 0
6 0 0
7 0 0
8 0 0
9 0 0
```

7. Analyze the result by executing

/home/qigui/ovito-2.8.0-x86_64/bin/ovitos ws_for_linux.py

8. When you see “finished” on the screen, the analysis is over.
9. Now you get files named as “nnws_analysis_fin”. They contain the number of vacancies and interstitials in each steps
10. In the next slide, more details of the instruction will be shown.

Remember, the analysis is based on OVITO program, so you need to execute the python script with “/home/qigui/ovito-2.8.0-x86_64/bin/ovitos ws_for_linux.py”

Details

```
#run a cascade simulation of Fe
#define variables here
variable Epka index 14 16 18 #add more energies here like in the example but expand the energy
#random seed generator, change the number 190900 to any other positive integers to get your own
variable seed equal 190900+${Epka}
```

1. You can change the numbers (14,16,18…) to wider or narrower energy range, bigger or smaller intervals to control the PKA energy.
2. Change the random seed 190900 to any other positive integers to get different simulation. With the same random seed and PKA energy, the simulations are always the same.

Details

```
14  #atom definition
15  lattice bcc 2.855312000
16  region unit cell block 0 9 0 11 0 9 #
```

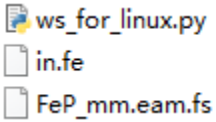
```
65  variable va equal 107.32782176636427*sqrt(${Epka}/100)
66  variable vb equal 1.0*${va}
67  variable vc equal 1.0*${va}
68  velocity pka set ${va} ${vb} ${vc} units box  #135 direction
69  #v in x,y,z directions, unit is angstrom/ps
```

3.Cell size is 9*11*9. Too small sizes are not good to calculate threshold energy.

4. The velocity and direction of 111 direction are defined here. My way of doing it:

a) Calculate the velocity of Fe atom with 100 eV kinetic energy (V1).
b) Project V1 on x axis (Va)
c) Va*sqrt(PKA/100) is the velocity of a given PKA energy on x axis (PKA=14, 16…).
d) Calculate Vb and Vc, you get velocity on y and z axis
e) Think about how to calculate PKA energy for 135 or other directions.

```
variable  = ['14','16','18']
path_to = '/home/qigui/lammps/lammps-22Aug18/test/md-lab-test/111/' #change this path
```



5. When analyzing the results, you need to specific the path of your result.
“path_to” is the path where you store your calculation with various directions. In our case, it is the folder containing 100,110,111 directions. To get the path, go to the directory and enter the command “pwd”, you can then copy the path to the variable path_to (and path_to must end with a “/”).
Variable (I know it’s a bad variable name) contains the PKA energy. Remember to edit it when you edited the PKA energy ranges in input file

Example: I have a new folder named “1_3_5” for 135 direction, the pka energy is (30,40,50…190, 200 eV). I only want to analyze the result in this new folder, what do I do?
Answer: Copy python script to the folder. Change “variable" to [‘30’,’40’,….’190’,’200’]. Change “path_to” to “/path/to/new/folder/1_3_5/”. Execute the script.
Remember, the analysis is based on OVITO program, so you need to execute the python script with “/home/qigui/ovito-2.8.0-x86_64/bin/ovitos ws_for_linux.py”