



ROYAL INSTITUTE  
OF TECHNOLOGY

# LAB: Point defects

## *Molecular dynamics simulations*

Pär Olsson & Ebrahim Mansouri

[polsson@kth.se](mailto:polsson@kth.se)

0737-650538

Nuclear Engineering

KTH – AlbaNova, Stockholm, Sweden

## Logging in to the server



ROYAL INSTITUTE  
OF TECHNOLOGY

### File transfer from your computer:

Use e.g. FileZilla or WinSCP  
(both free)

Make sure to edit input files  
directly **on the server**, not on  
your windows machine.

Output: use as you like!

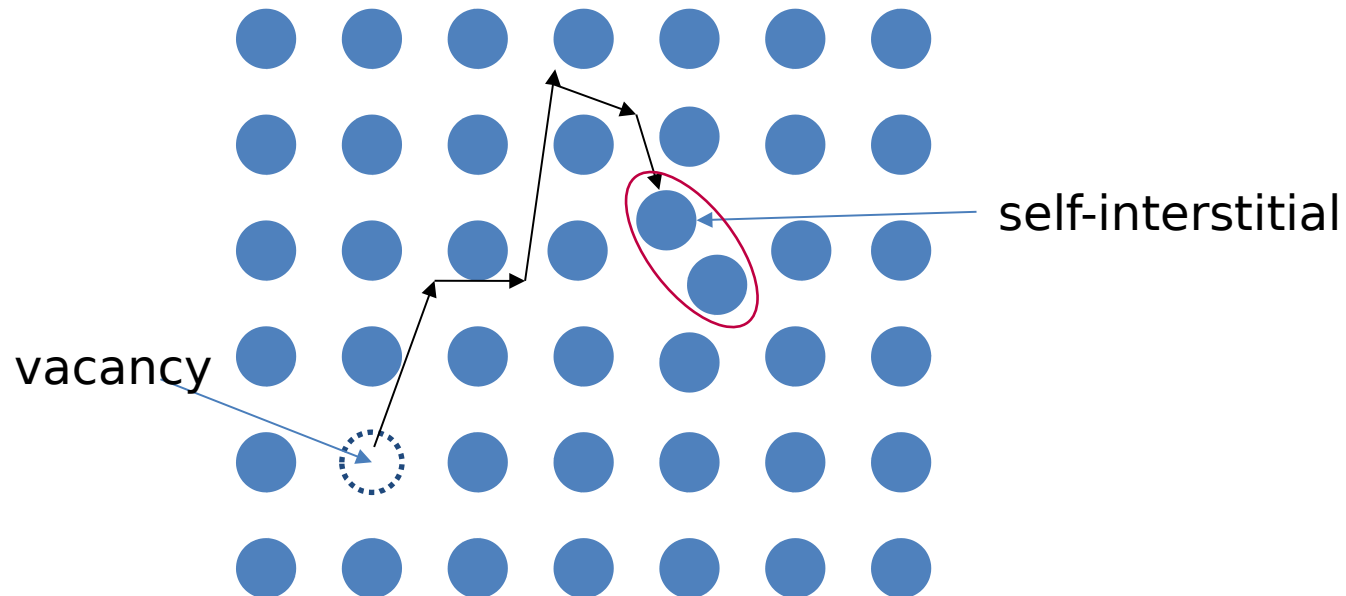
- The server is running ubuntu
- ssh to 130.237.70.27
- Username: sh2605
- Password: SH2605
  - Do not spread IP, username or password (do not email about them, SMS, Whatsapp, whatever, please...)
- Login and enter the folder MD
  - cd MD
- Then enter the folder with your name
  - cd Yourname (e.g. cd Par for me)
- There you have all the initial files, the executables etc
  - To see files: ls (or ls -l)
  - To edit files: nano file

# Elastic scattering – point defects

A fast neutron interacts with matter and displaces an atom from its equilibrium lattice site:

- What is the maximum kinetic energy of an Fe atom hit by a 1 MeV neutron?  
( $E_{in} = E_{out}$  ;  $P_{in} = P_{out}$ )

If the atom is given a large enough impulse, it will leave its place in the lattice and create a Frenkel pair, i.e. a vacancy and a self-interstitial.



ROYAL INSTITUTE  
OF TECHNOLOGY

# LAMMPS



ROYAL INSTITUTE  
OF TECHNOLOGY

Description of the simulation in an input file name.in

- interaction potential (cohesive model)
- crystal
- definition of output files
- simulation (minimization (e.g. quench), molecular dynamics, ...)
- analysis of results

To run:

- `lammps < name.inp`
- `lammps < name.in > name.out`

To get the wanted information:

- `grep "flag" name.out`
- or check the other output files!

Example of a simple quench algorithm:

if scalar product of velocity and displacement  $< 0$   
then set velocity = 0

## a) Lattice parameter



ROYAL INSTITUTE  
OF TECHNOLOGY

1. Read an EAM potential for Fe
2. Construct a crystal
3. Calculate the energy as a function of the lattice parameter

- What is the equilibrium lattice parameter of Fe?
- What is the cohesive energy of Fe?

You may need to change the interval and stepping to "zoom in" on the equilibrium

*Extra: Use the `input.rose.in` to plot the Rose curve → more complete equation of state*

## b) Vacancy

Create a vacancy by removing one atom



ROYAL INSTITUTE  
OF TECHNOLOGY

- What is the formation energy of a vacancy?
  - Unrelaxed?
  - Relaxed?
  - What is the effect of relaxation on  $E_{\text{formation}}$ ?

What is the vacancy concentration at 300K, 600K, 900K, 1200K? (from theory, with this  $E_f$ )

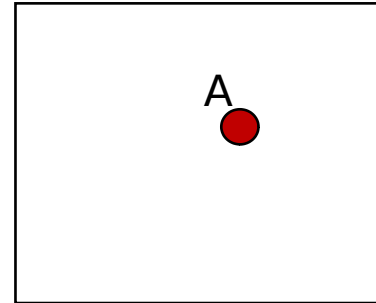
# Formation energy



ROYAL INSTITUTE  
OF TECHNOLOGY



- N atoms
- $E_{\text{ref}}$



- Vacancy: (N - 1) atoms:  $E_{\text{vac}}$
- Self-interstitial: (N+1) atoms:  $E_{\text{int}}$

Two cases:

1. Relaxation
2. Static calculation

$$E_{\text{for}}(\text{vac}) = E_{\text{vac}} - E_{\text{ref}}(N - 1)/N$$

$$E_{\text{for}}(\text{int}) = E_{\text{int}} - E_{\text{ref}}(N+1)/N$$

## c) Di-vacancy

Create a vacancy by removing one atom,  
then a second one in first nearest neighbour position

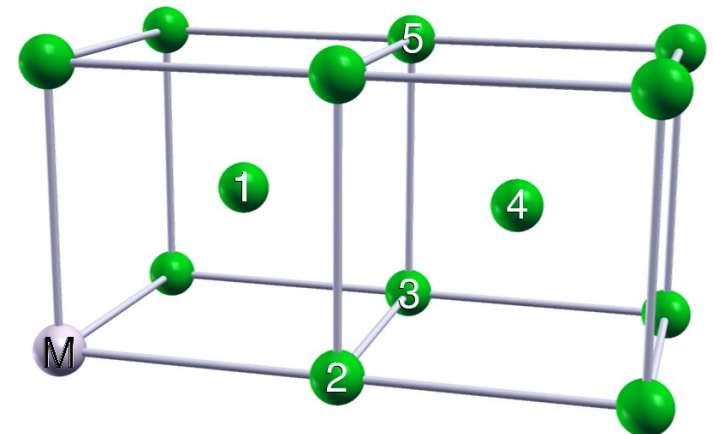
- What is the formation energy of the di-vacancy?
- What is the binding energy of the di-vacancy?



ROYAL INSTITUTE  
OF TECHNOLOGY

Change the input in order to setup 2<sup>nd</sup>, 3<sup>rd</sup>, etc nearest  
neighbour di-vacancies

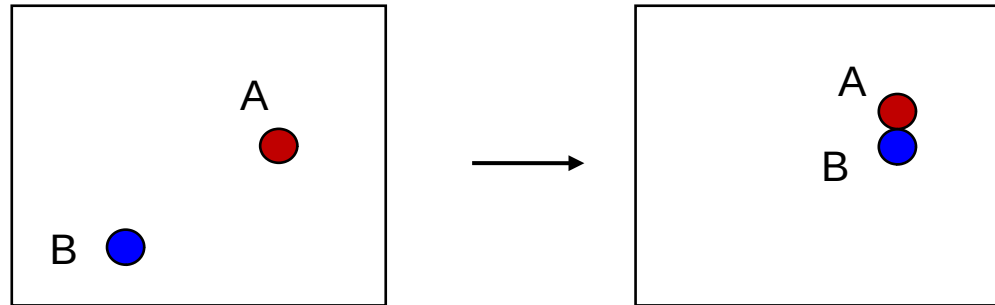
- What is the binding energy of the 2nn di-vacancy?
- What is the binding energy of the 3nn di-vacancy?
- How far do you have to separate the  
vacancies to have zero interaction?  
(4nn, 5nn, ...)





# Binding energy

Definition:



$$E_{\text{binding}} = E(\text{defects A and B far separated}) - E(\text{defects A and B close})$$

$E_{\text{binding}} > 0$  : attraction ;  $< 0$  : repulsion

Alternate way of calculating binding energy:

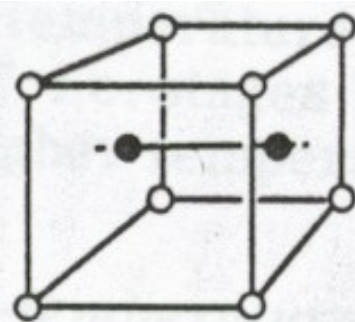
$$E_{\text{binding}} = \left( \begin{array}{|c|} \hline \text{A} \\ \hline \end{array} \right) + \left( \begin{array}{|c|} \hline \text{B} \\ \hline \end{array} \right) - \left( \begin{array}{|c|} \hline \text{A} \\ \hline \text{B} \\ \hline \end{array} \right) + \left( \begin{array}{|c|} \hline \\ \hline \end{array} \right)$$

## d) Self-interstitial defect configurations

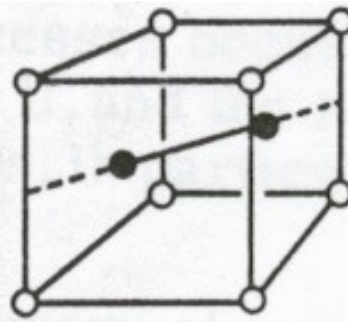
Example: self-interstitial configurations in bcc Fe



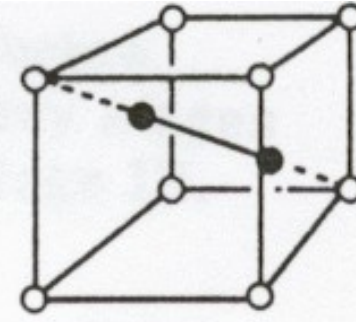
ROYAL INSTITUTE  
OF TECHNOLOGY



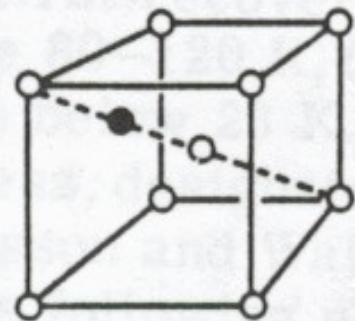
(a) **<100>**



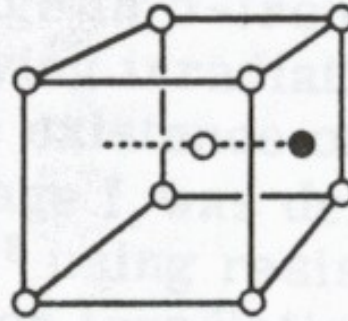
(b) **<110>**



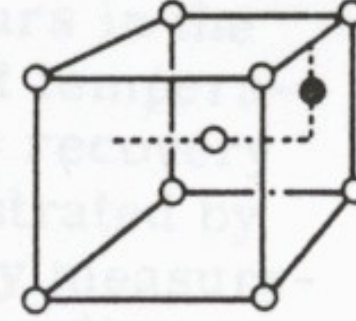
(c) **<111> dumbbell**



(d) **<111> crowdion**



(e) **(O)**



(f) **(T)**

## d) Self-interstitials

Create a  $\langle 110 \rangle$  self-interstitial

- What is the formation energy?
- What is the *effect* of relaxation? (geometrically)



ROYAL INSTITUTE  
OF TECHNOLOGY

Copy the input to a new file

Modify it in order to create  $\langle 111 \rangle$  and  $\langle 100 \rangle$  interstitials

- What are the formation energies?
- Which configuration is the most stable?

Compare to the formation energy of a vacancy

- What is the self-interstitial concentration at 300K, 600K, 900K, 1200K? (from analytical theory, with these values)

## e) Threshold energy



ROYAL INSTITUTE  
OF TECHNOLOGY

Estimate the threshold energy for a stable Frenkel pair in Fe.

- How do the different crystal directions differ?  
(Investigate  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ ,  $\langle 135 \rangle$ )

Why should one take care not to use a cubic simulation cell for the  $\langle 111 \rangle$  direction?