Friedrich-Alexander-Universität
Naturwissenschaftliche Fakultät

FAU

DISCUS Workshop

Single crystal disorder

Stacking faults

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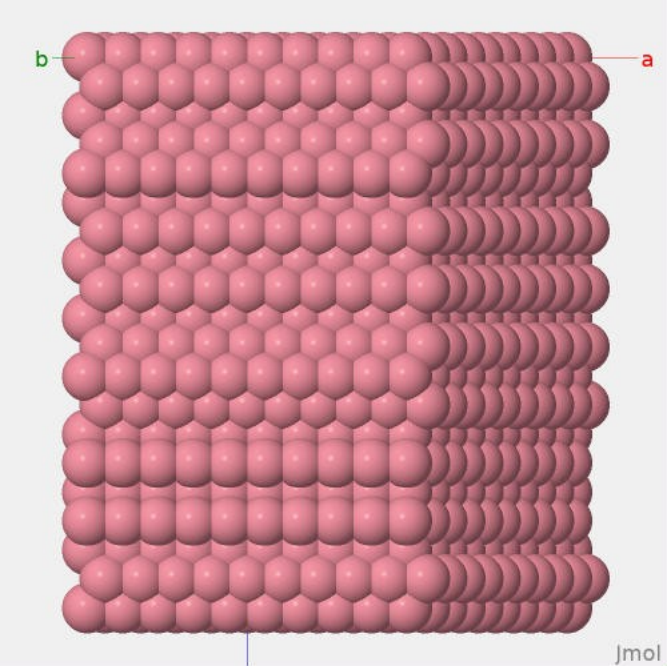
Stacking faults



Goal:

Build a 3D crystal with stacking faults

Basic Info:

Layer types

Layer sequence

A quick demonstration

Stacking faults

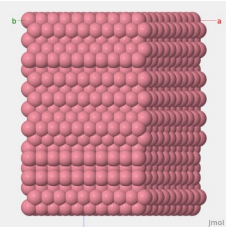
Open in Windows Explorer: Lectures\ 09_Stacking_Faults\ STACK_01

Start DISCUS_SUITE

You should see:

...
User macros in ...
System macros in ...
Start directory ...

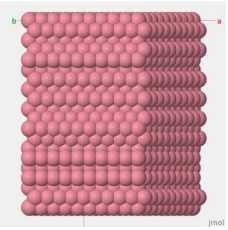
suite >



suite > **cd Lectures\09_Stacking_Faults\STACK_01**

suite > **@stack_01.mac 0.00**

Stacking faults



Stacking faults

Open in Windows Explorer: Lectures\ 09_Stacking_Faults\ STACK_01

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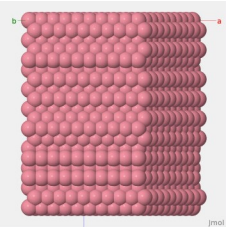


suite > **cd Lectures\09_Stacking_Faults\STACK_01**

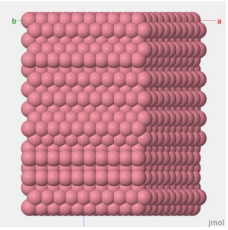
suite > **@stack_01.mac 0.00**

Try different probabilities

Stacking faults

stack_01.mac

```
discus
#
read
  cell  hexagonal.cell,10,10, 1
#
save
  outfile hexagonal.layer
  run
exit
```



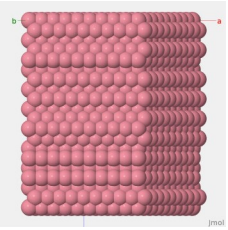
Build and save individual layers

- Build 2D-Layers
- Cut layers out of a large structure

Stacking faults

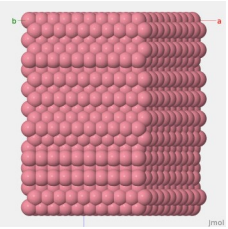
stack_01.mac

```
stack
#
  layer  hexagonal.layer
  layer  hexagonal.layer
```



The Cobalt structure will consist of two (identical) layer types

Stacking faults



stack_01.mac

```
stack
#
  layer  hexagonal.layer
  layer  hexagonal.layer
  trans  1,1, 1./3.,-1./3., 1./2
  trans  1,2,-1./3., 1./3., 1./2
  trans  2,1, 1./3.,-1./3., 1./2
  trans  2,2,-1./3., 1./3., 1./2
```

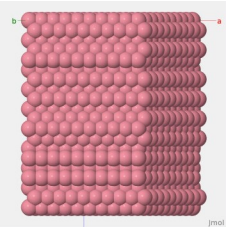
The Cobalt structure will consist of two (identical) layer types

Translation vectors from **first** layer type to **second** layer type need to be defined
components in fractional coordinates in direct space

Stacking faults

stack_01.mac

```
stack
#
  distr  matrix
  first  random
  crow   1,     $1       , 1.00-$1
  crow   2,     1.00-$1, $1
  number 20
```



The layer **distribution** is determined by the **matrix** with commands **crow**

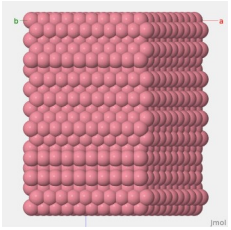
For each row the elements specify probability for the current layer type (**row index**)
to be
followed by next (column index)

20 layers will be stacked, the first is of **random** layer type

Stacking faults

stack_01.mac

```
stack
#
  aver    0.00, 0.00, 1.00
  modul   1.00, 0.00, 0.00, 0.00, 1.00, 0.00
  set     modulus,on
  set     trans,fixed
```



A quick demonstration
Turn off:
set modulus , off

@stack_01.mac 1.0

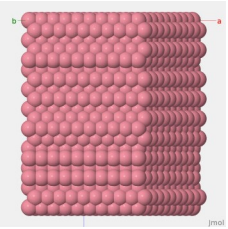
The average growth direction shall be [0, 0, 1]

Shift layers back to [001] by the two modulus vectors

Stacking faults

```
stack
#
   create
   run
exit
```

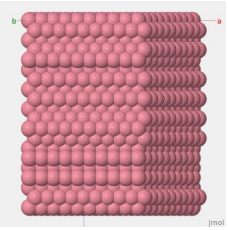
stack_01.mac



A quick demonstration
Turn off:
set modulus , off

@stack_01.mac 1.0

First **create** list of origins only

With **run** place actual atoms into the crystal

Stacking faults