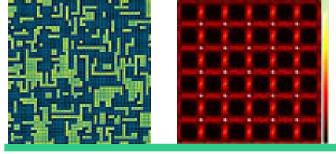
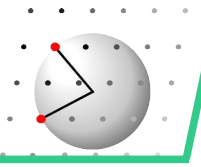


tutorial session I

simulation of a crystal structure



Simulate a crystal structure

Open in Windows Explorer: Lectures\01.Simulation

Start DISCUS_SUITE

DISCUS_SUITE
needs to be in correct folder

type: suite > cd

Left click on folder icon
Full path will be in blue
Copy with CTRL c
Activate DISCUS_SUITE Window
Paste by SHIFT + right mouse button

suite > cd c:\Users...\01.Simulation

You should see:

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

suite >

NO RETURN YET !!

HIT RETURN

perfect crystal structure

List of:

all atom positions
type, x,y,z, U/B

sequence ?

Minimum information needed to create

space group

unit cell dimensions

Content of asymmetric unit
list of all atoms:
type x,y,z, U/B

size of the crystal

```
title  zirconia in Fm-3m
spcgr  Fm-3m
cell   5.14, 5.14, 5.14, 90.0, 90.0, 90.0
atoms
Zr   0.000000,  0.000000,   0.000000,  0.8
O    1./4.   ,  0.250000,   0.250000,  0.8
```

1. Task: a 1D crystal

Start DISCUS section — discus

You should see:

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

suite > discus
discus>

within DISCUS type — read
cell primitive.cell

Information on unit cell ...

show atom , all

just one atom: Po at 0,0,0

```
discus > show atom,all
Name            x             y             z             B
PO(1)           0.000000      0.000000      0.000000        1.000000
discus >
```

within DISCUS type — read
cell primitive.cell, 5,1,1

show atom , all

2. Task: a 2D crystal and plot the structure

make sure you your prompt says discus>

Otherwise start DISCUS: discus

Verify folder: system pwd

Should be: **c:\Users...\01.Simulation**

within DISCUS type:
read
cell primitive.cell, 3, 3, 1

@plot.mac 2d

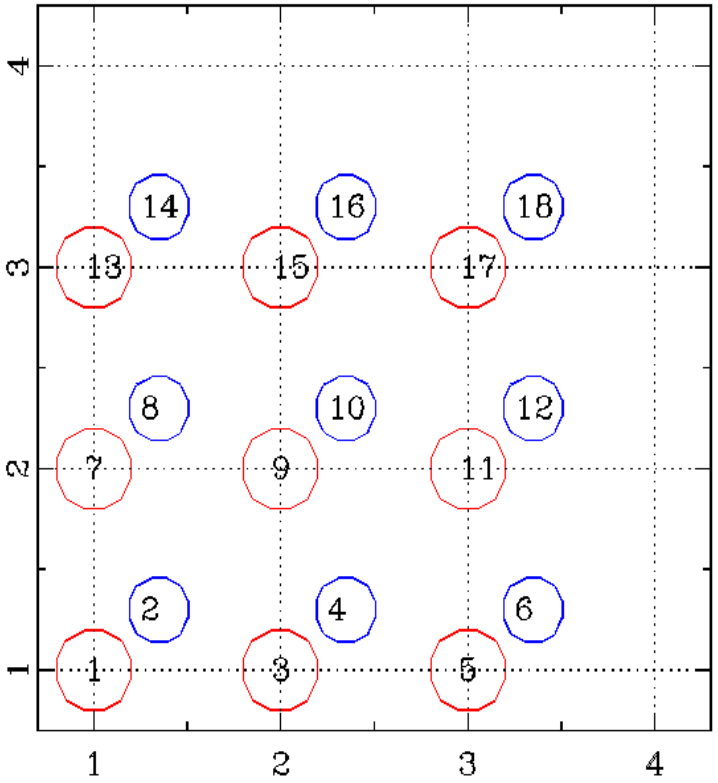
show atom , all

start KUPLOT: branch kuplot

within KUPLOT type: @kplot.mac 2d

within KUPLOT type: exit

Y - axis



X - axis

Seqence of atoms in perfect:

Within each unit cell == sites

Unit cells along x

Unit cells along y

Unit cells along z

All **red** atoms on site 1
All **blue** atoms on site 2

3. Task: a 3D crystal and plot the structure

make sure your prompt says discus>:

Otherwise start DISCUS

```
discus
```

```
discus
```

within DISCUS type

```
read
cell primitive.cell, 3, 3, 3

@plotcif.mac 3d

show atom , all
```

Starts an interactive jmol

4. Task: a 2D crystal modification of atoms

make sure your prompt says discus>:

Otherwise start DISCUS: discus

within DISCUS type:

```
read
cell primitive.cell, 5, 5, 1

x[13] = 0.5
y[13] = 0.5
replace 13, Zr, 1.0

@plot.mac modified

show atom , all
```

start kuplot: branch kuplot

within KUPLOT type:

```
@kplot modified
exit
```

5. Task: a 2D crystal inserting individual atoms

make sure your prompt says

DISCUS

discus>:

KUPLOT

read
free 5.0, 5.0, 5.0, 90.0, 90.0, 90.0

An empty cubic space is defined with a=5 Å

branch kuplot

insert po, 0, 0, 0, 0.8
insert po, 0, 1, 0, 0.8
insert po, 0, 2, 0, 0.8
insert po, 1, 0, 0, 0.8
insert po, -1, -1, 0, 0.8

A single Po atom is inserted at 0,0,0 with B=0.8

@plot.mac modified

show atom, all

Atoms are now in sequence as typed !

@kplot modified
exit

6. Task: a 2D crystal; modification of atoms

make sure your prompt says discus>:

DISCUS

```
read
cell primitive.cell, 5, 5, 1

do i[0]=1, n[1], 1
  if( mod( i[0], 3 ) == 0 ) then
    replace i[0], Zr, 1.0
  elseif( mod( i[0], 3 ) == 1 ) then
    remove i[0]
  endif
enddo

@plot.mac  changed

chemistry
  element
exit

show atom , all
```

Loop from 1 to number of atoms
  if at atom 3, 6, 9, ...
    replace by a Zr atom with B=1.0
  otherwise if at atom 1, 4, 7, ...
    remove atom from crystal

write crystal for plotting

go to chemistry menu
  check stochiometry
exit the chemistry menu

removed atoms are just replaced by voids!

KUPLOT

```
branch kuplot

@kplot changed
exit
```

7. Task: a 2D crystal; symmetry operation

make sure your prompt says discus>:

DISCUS

```
read
cell cmm2.cell,3,2,1
@plot.mac  molecule

symmetry
  uvw     0, 0, 1
  angl    30.0
  trans   0, 0, 0
  type    proper
  power   1,single
  mode    repl,new
  orig    0, 0, 0, mol

  msel 1
  minc 17, 20

  show
  run
exit
@plot.mac  molecule
```

Branch to symmetry menu
- symmetry axis is [0, 0, 1]
- rotation angle is 30.0°
- translation part is [0, 0, 0]
- proper rotation, not rotoinversion
- apply rotation once, single result
- replace the object, create a new type
- origin is at [0,0,0] with respect to molecule

- select molecules of type 1
- includes molecule no. 17 through no. 20

- show parameters for symmetry operation
- execute symmetry operation

exit the symmetry menu
plot the modified crystal

KUPLOT

```
branch kuplot
@kplot molecule
exit
```

```
branch kuplot
@kplot molecule
exit
```

DISCUS	blen(u,v,w)	length of vector [u, v, w]
	blen(u,v,w, o,p,q)	length of vector [u, v, w] – [o, p, q]
	blen(atom, i, j)	length of vector between atoms no. i and j
	bang(u,v,w, o,p,q)	angle between vectors [u, v, w] and [o, p, q]
	bang(atom,i, j, k)	bond angle in atom j between i-j and k-j
	dstar(h,k,l)	length of reciprocal vector [h, k, l]
	rang(h,k,l, m,n,o)	angle betwen reciprocal vectors [h, k, l] and [m, n, o]
	scalpro(u,v,w, o,p,q, flag)	scalar product of vectors [u, v, w] and [o, p, q] flag signals whether vectors are from direct or reciprocal space, or mixed

---

vprod u,v,w, o,p,q, flag	vector product of vectors [u, v, w] and [o, p, q] flag signals whether vectors are from direct or reciprocal space, or mixed

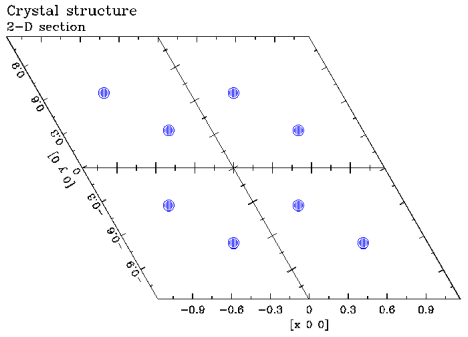
Pit falls

Edit file „hexagonal.cell“

```
title hexagonal
spcgr P63mc
cell    3.00   3.00   4.8989797   90.00   90.00   120.00
atoms
co      0.333333   0.6666667   0.0000    1.0
```

discus>
```
read
cell hexagonal.cell,2,2,1
@plot.mac  hexagonal
read
cell hexagonal.cell
show atom ,  all
```

kuplot>
```
branch kuplot
@kplot6.mac hexagonal
exit
```



Pit falls

Edit file „p6.cell“

```
title hexagonal
spcgr P6
cell    3.00   3.00   4.8989797   90.00   90.00   120.00
atoms
co      0.333       0.667        0.0000    1.0
```

discus>
```
read
cell p6.cell,2,2,1
@plot.mac p6
read
cell p6.cell
show atom ,  all
```

kuplot>
```
branch kuplot
@kplot6.mac p6

skal 0.66, 0.67, 0.33, 0.34
plot
exit
```

```
discus > show atom,all
Name            x             y             z             B
CO(1)           0.333000      0.667000      0.000000        1.000000
CO(1)           0.333000      0.666000      0.000000        1.000000
CO(1)           0.334000      0.667000      0.000000        1.000000
CO(1)           0.667000      0.333000      0.000000        1.000000
CO(1)           0.667000      0.334000      0.000000        1.000000
CO(1)           0.666000      0.333000      0.000000        1.000000
```

Homework 1

Create a circle of N atoms. The circle shall have radius R. Plot to verify

Homework 1

Create a circle of N atoms. The circle shall have radius R. Plot to verify

```
variable real, radius
variable real, angle
variable integer, number
variable integer, counter

radius   = $1
number = $2
angle    = 360.0/number

read
  free 1,1,1, 90, 90, 90

do counter = 1,number
  insert Zr,  radius*cosd(counter*angle),  radius*sind(counter*angle),  0.0,  0.55
enddo

@plot.mac circle

branch kuplot
@kplot.mac circle
exit
```