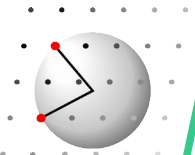




tutorial session XIII

Analyzing simulated disordered structures



A disordered structure might be the result of an RMC cycle

RMC: pretent to be blind and
 let the modify itself to fit to experimental data

What is the result, what characterizes the structure???

Any SRO ?

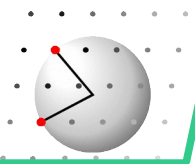
Any displacements ?

Any domains ?

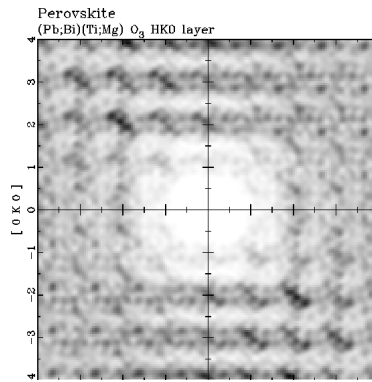
Any peculiarities in the local structure ?

ETC ETC ETC

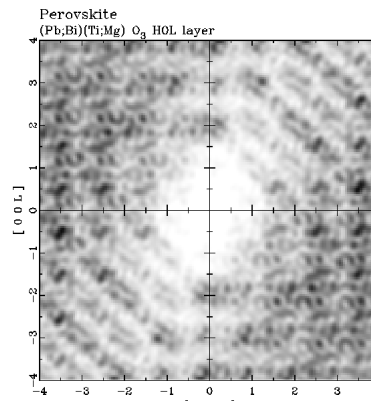
Chemistry menu to the rescue



Diffuse pattern of a disordered Perovskite

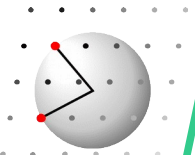


H 0 L layer



H 0 L layer

What is the local structure?



Exercise 1



Start discus_suite
Select directory Lectures\13.Analyze

suite> **discus**

discus> **read STRU/perovskite.stru**

discus> **show metric**

discus> **show metric**

Pm-3m 221

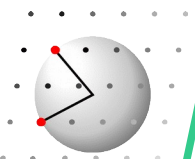
Lattice constants :

a	b	c
3.95000	3.95000	3.95000 ...

Current crystal dimensions:

	minimum	maximum
X	-0.2111	9.5820
Y	-0.1709	9.5957
Z	-0.1062	9.6212

Crystal size in unit cell dimensions





Start `discus_suite`

Select directory `Lectures\13.Analyze`

`discus> chemistry`

`discus/chem> element`

```
Size of the crystal (unit cells) : ...
Total number of atoms           : ...
Number of atoms per unit cell   : ...
Number of different atoms       : ...
```

Element : VOID(0) rel abundance

Information on the elements present in
the current structure

Information on the average crystal structure

how many different sites in the unit cell,
what is the average position
what is the average atomic displacement
what is the occupancy

Results are stored in `res[1]`, `res[2]`, ...

`discus/chem> aver`

`discus/chem> aver ind`



Start discus_suite

Select directory Lectures\13.Analyze

discus/chem> **set blen, 1.5, 2.5**

discus/chem> **set bin, 100**

discus/chem> **blen Ti, O, CHEM/ti_o.hist**

Define an allowed Bond length range
Set number of blen intervals
Determine Ti-O bond length distribution,
write output to file CHEM/ti_o.hist
(Directory must exist!)

discus/chem> **set blen, 0.5*lat[1]-0.5, 0.5*lat[1]+0.5**

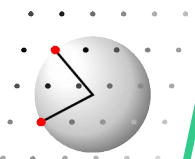
discus/chem> **set bang, 1.0, 180.0**

discus/chem> **set bin, 179**

discus/chem> **bang Ti, N, N, CHEM/ti_nn.hist**

TiO distance is 1/ lattice parameter
Define an interval

Determine Bond angle distribution



Exercise 1



```
discus/chem>
```

```
set neig,rese
```

```
set vec, rese
```

```
set vec, 1, 1, 1, 1, 0, 0
```

```
set vec, 2, 1, 1, -1, 0, 0
```

```
set vec, 3, 1, 1, 0, 1, 0
```

```
set vec, 4, 1, 1, 0, -1, 0
```

```
set vec, 5, 1, 1, 0, 0, 1
```

```
set vec, 6, 1, 1, 0, 0, -1
```

```
set nei, vec, 1, 2, 3, 4, 5, 6
```

```
corr occ, Pb,Bi
```

Reset all neighbor and vector definitions

Set several vectors here:

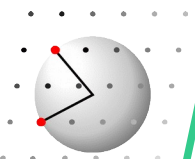
From site **1** to site **1** in the unit cells

Offset by **$[\pm 1, 0, 0]$, $[0, \pm 1, 0]$, $[0, 0, \pm 1]$**

Group six vectors to a neighborhood

Determine chemical short range order

Correlation between Pb and Bi

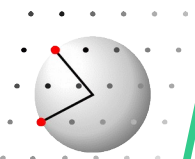


Exercise 1



Start discus_suite
Select directory Lectures\13.Analyze

suite> [@analyze.mac](#)



Exercise 1

