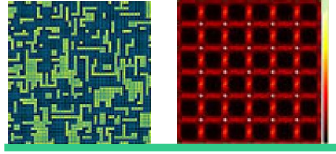
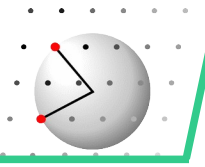


tutorial session XI

Analyzing simulated disordered structures



Lehrstuhl für Kristallographie und Strukturphysik
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A disordered structure might be the result of an RMC cycle

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

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

Any SRO ?

Any displacements ?

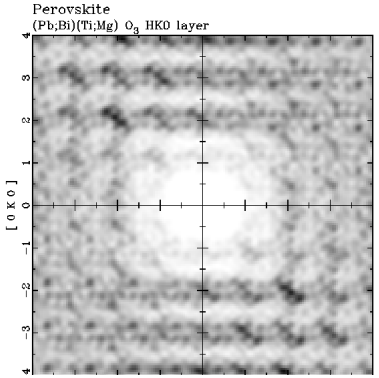
Any domains ?

Any peculiarities in the local structure ?

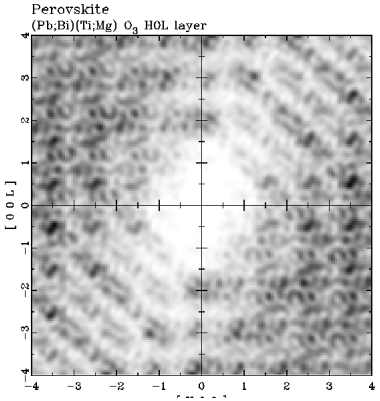
ETC ETC ETC

Chemistry menu to the rescue

Diffuse pattern of a disordered Perovskite



H 0 L layer



H 0 L layer

What is the local structure?

Start discus_suite
Select directory Lectures\11_Analyze

suite> **discus**
discus> **read**
discus/read> **stru STRU/perovskite.stru**
discus> **show metric**

discus> **show cdim**

```
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\11_Analyze

```
discus> show symmetry, symbol
Space group Pm-3m  No.: 221 cubic
Symmetry No. [  3]      Number as in International Tables
            (  3)      Number within centering group
              *        Point group element (omit translation)
             3P        Symmetry symbol
                       If present translation vector
        0, 0, +z       Position within unit cell
             GEN       This element is a Generator
               F       This is a centering vector
               2       Number as in International Tables
```

Try:

```
suite> discus
discus> read
discus/read> free  1, 1, 1,  90,90,90,  different_space_groups
discus/read> show symmetry,    { symbol  |  matrix |  full }
```

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 diferent atoms          : ...

   Element : VOID(0)    rel abundance
```

Information on the elements present in the current structure

discus/chem> **aver**

Information on the average crystal structure

discus/chem> **aver ind**

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], . . .

Start discus_suite
Select directory Lectures\13.Analyze

discus/chem> **set blen, 1.5, 2.5**
Define an allowed Bond length range

discus/chem> **set bin, 100**
Set number of blen intervals

discus/chem> **blen Ti, O, CHEM/ti_o.hist**
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**
TiO distance is 1/ lattice parameter

discus/chem> **set bang, 1.0, 180.0**
Define an interval

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

discus/chem> **bang Ti, N, N, CHEM/ti_nn.hist**
Determine Bond angle distribution

```
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 **[±1,0,0], [0,±1,0], [0,0,±1]**

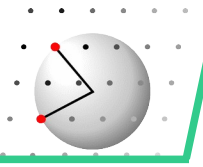
Group six vectors to a neighborhood
Determine chemical short range order
Correlation between Pb and Bi

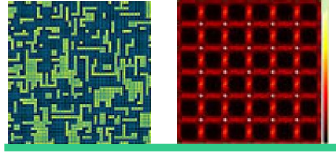
Start discus_suite
Select directory Lectures\13.Analyze

suite> **@analyze.mac**

Start discus_suite
Select directory Lectures\13.Analyze

suite> **@chem_homo.mac Pb, 5**





Exercise 1