Friedrich-Alexander-Universität
Naturwissenschaftliche Fakultät

DISCUS Workshop

Single crystal disorder

Chemical short range order

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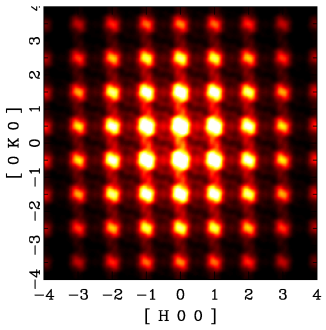
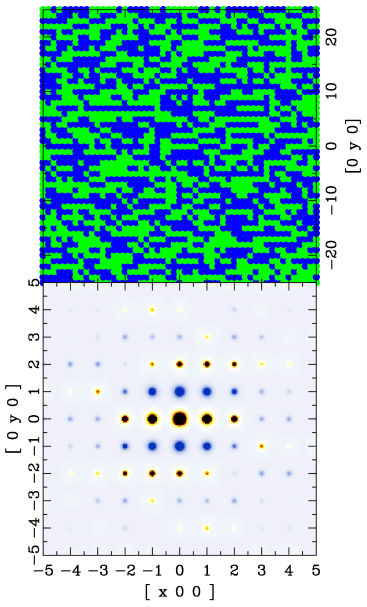
Short range order





C100 target/achieved/ 0.30 0.30
C010 target/achieved/−0.20 −0.21
C110 target/achieved ..... −0.12
CM10 target/achieved ..... −0.10
temperature 1.0
copper : gold 0.50 : 0.00

Goal:

Build a 2D/3D crystal

Introduce chemical short range order

Calculate 3D-PDF

Basic Info:

Short range order parameters

A quick demonstration

Short range order

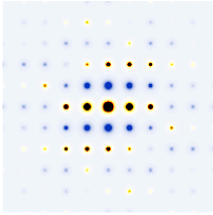
Open in Windows Explorer: Lectures\08_Short_Range_Order\SRO_2

Start DISCUS_SUITE

You should see:

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

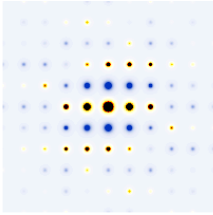
suite >



suite > **cd Lectures\08_Short_Range_Order\SRO_2**

suite > **@sro_2.mac -0.3, -0.3, 2.5**

Short range order



Short range order

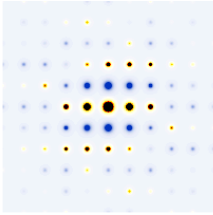
Open in Windows Explorer: Lectures\
08_Short_Range_Order\
SRO_2

Start DISCUS_SUITE

You should see:

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

suite >



suite > **cd Lectures\08_Short_Range_Order\SRO_2**

suite > **@sro_2.mac -0.3, -0.3, 2.5**

Try different parameter combinations

1st parameter : correlation along [1 0 0]

2nd parameter : correlation along [0 1 0]

3rd parameter : temperature kT

Short range order

Open in Windows Explorer: Lectures\
08_Short_Range_Order\
SRO_3

Start DISCUS_SUITE

suite > **cd Lectures\08_Short_Range_Order\SRO_3**

suite > **@sro_3.mac 0.50, -0.3, -0.3, 0.2, 0.2, 2.5**

Try different parameter combinations

1st parameter : composition]

2nd parameter : correlation along [1 0 0]

3rd parameter : correlation along [0 1 0]

4th parameter : correlation along [1 1 0]

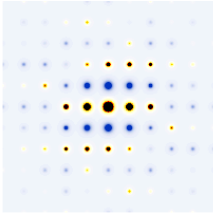
5th parameter : correlation along [1 $\bar{1}$ 0]

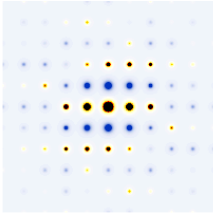
6th parameter : temperature kT

You should see:

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

suite >



Be creative!

Short range order