tutorial session IV

short range order
SRO

Short range order SRO

in disordered crystals “objects” are often ordered only at a short range distance

neighbours are not strictly periodic but present only with a given probability

example in 1-D chain

A A A B A **B** A B A A A B B A A B B B B A B

assumptions: objects are simple atoms
interatomic distances are strictly periodic

possible pairs are

AA with P_n^{AA}
AB with P_n^{AB}
BA with P_n^{BA}
BB with P_n^{BB}

P_n^{ij} probability to find a pair ij
n= 1,2,... distance in n***a**

relative occupations: m_A and m_B $0 \le m_A \le 1$
$m_A + m_B = 1$

influence of probabilities on diffraction pattern ?
what does a structrure look like for different probabilities ?
is any value for the probabilities allowed ?
connection between probabilities and occupation with A / B ?

A A A B A **B** A B A A A B B A A B B B B A B

Pair- pair correlation terms describe the probability P_n^{AA}
independent of chemical composition

$C_n=(P_n^{AA}-m_A^2)/(m_A m_B)$ pair correlation coefficient for atoms at distance n

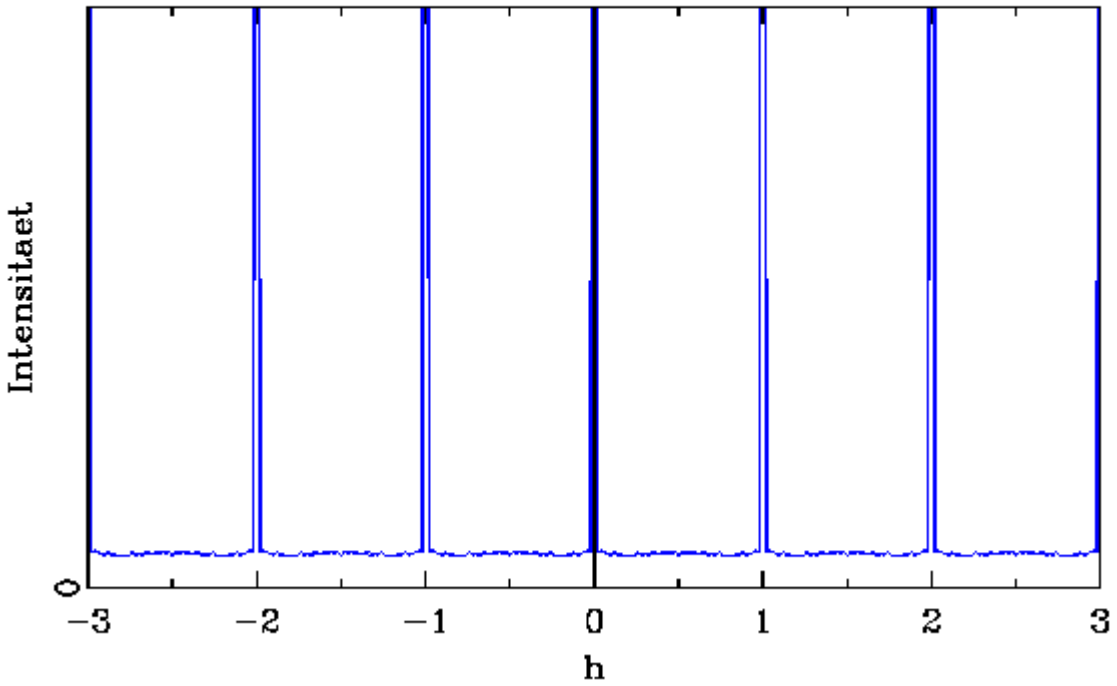
$C_n=0$ If distributed at random: $P_n^{AA} = m_A^2$

$C_n>0$ $P_n^{AA} > m_A^2$ preferably equal neighbors AA a*nd* BB

$C_n<0$ $P_n^{AA} < m_A^2$ preferably different neighbors AB a*nd* BA

$C_n = 0$ $m_A = 0.5$ random sequence

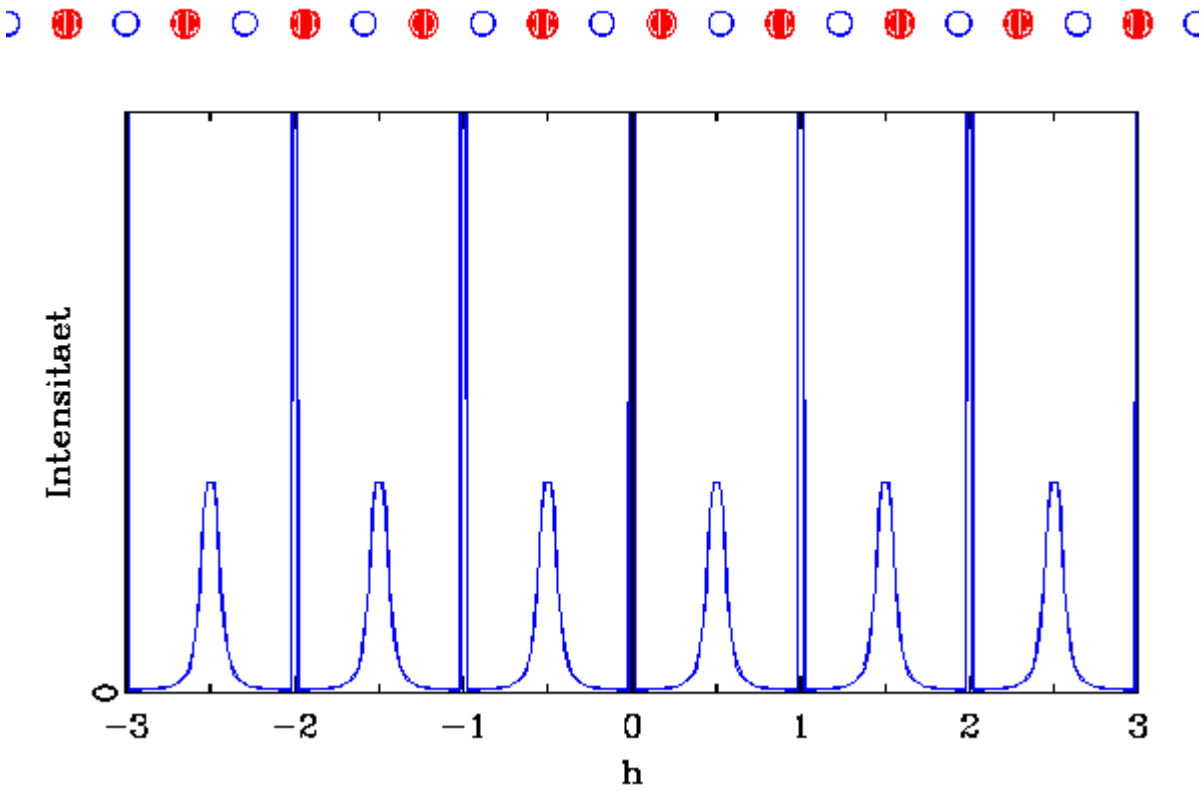
completey random seqence of the atoms



sharp Bragg peaks at integer h

simple continuous diffuse background

$C_n = -1$ $m_A = 0.5$



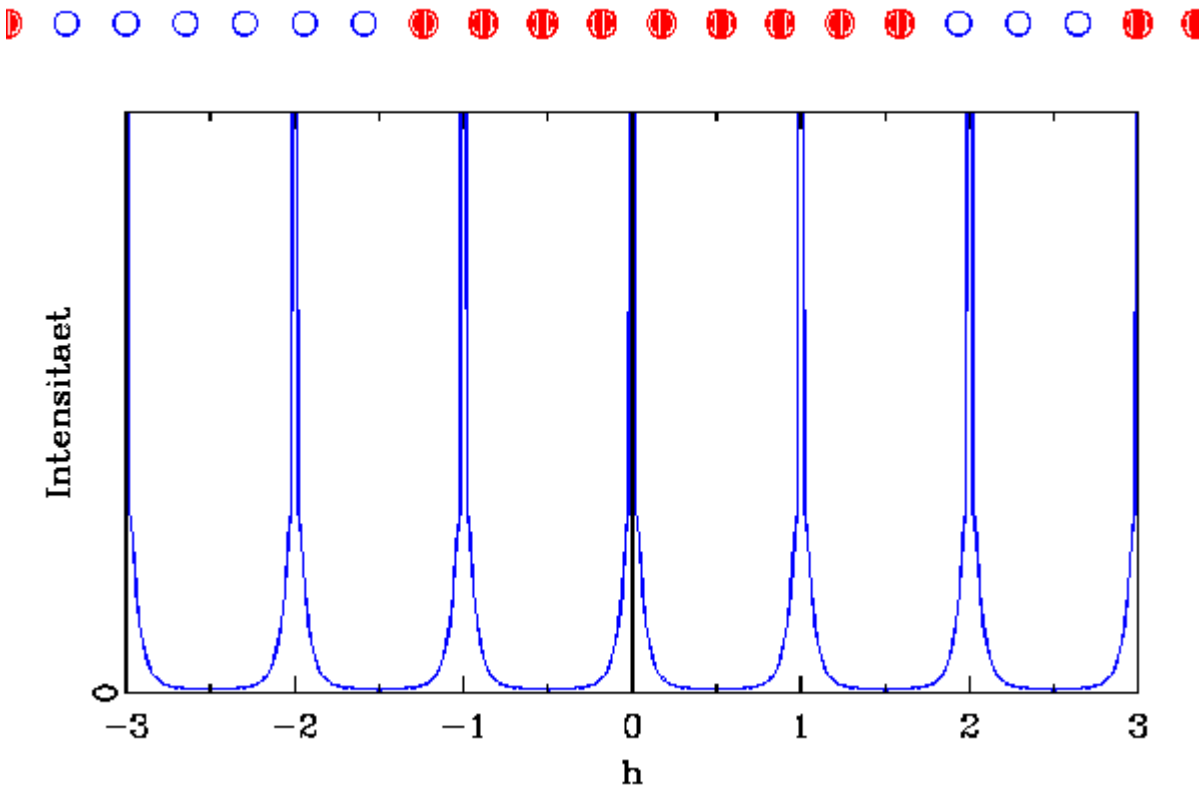
almost strict ABABABA sequence

sharp Bragg peaks at integer h

diffuse scattering maxima at h=1/2

Clear trend to form a period of 2**a**

$C_n = 1$ $m_A = 0.5$

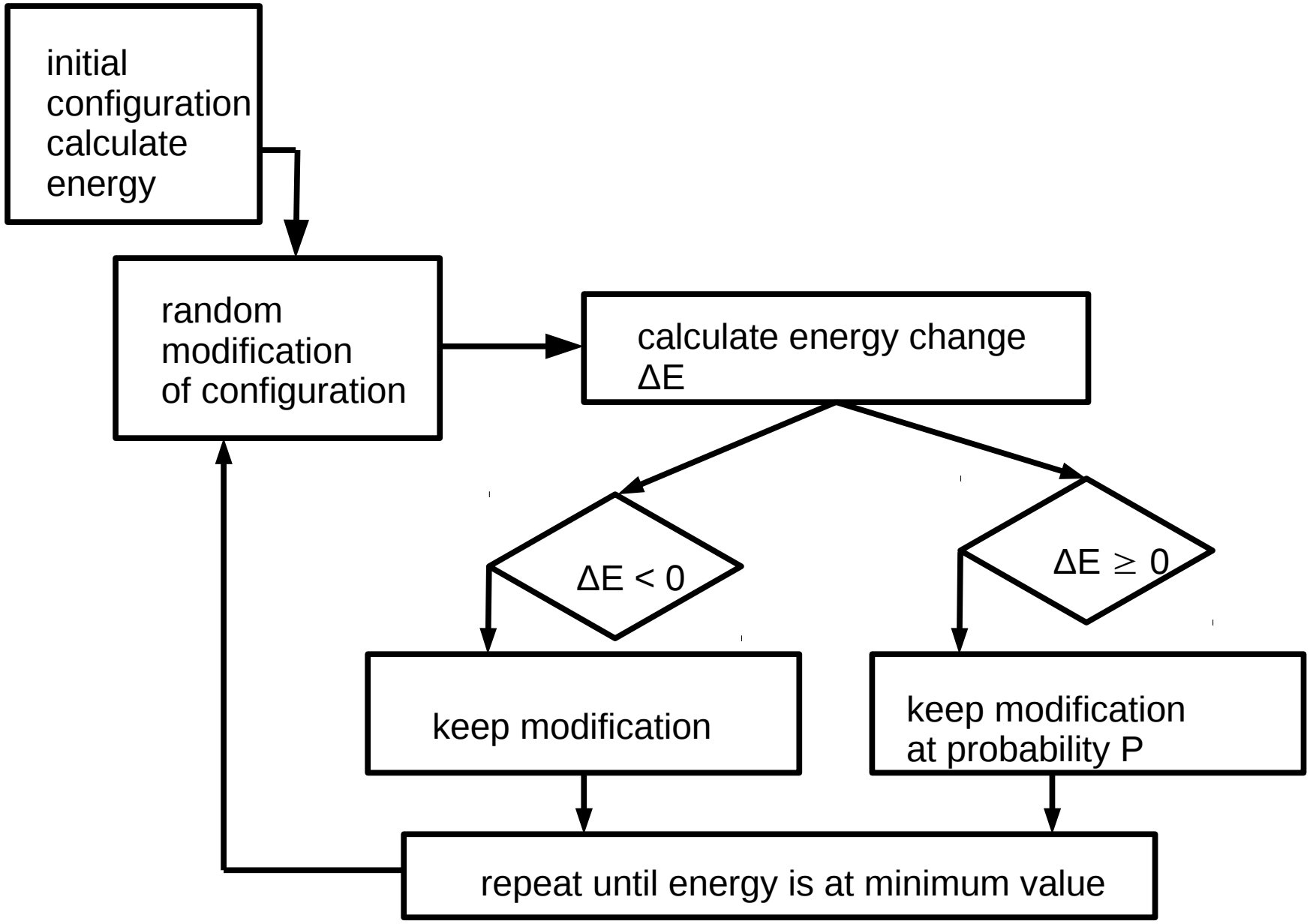


almost strict AAABBBA sequence

sharp Bragg peaks at integer h

diffuse scattering maxima at integer h

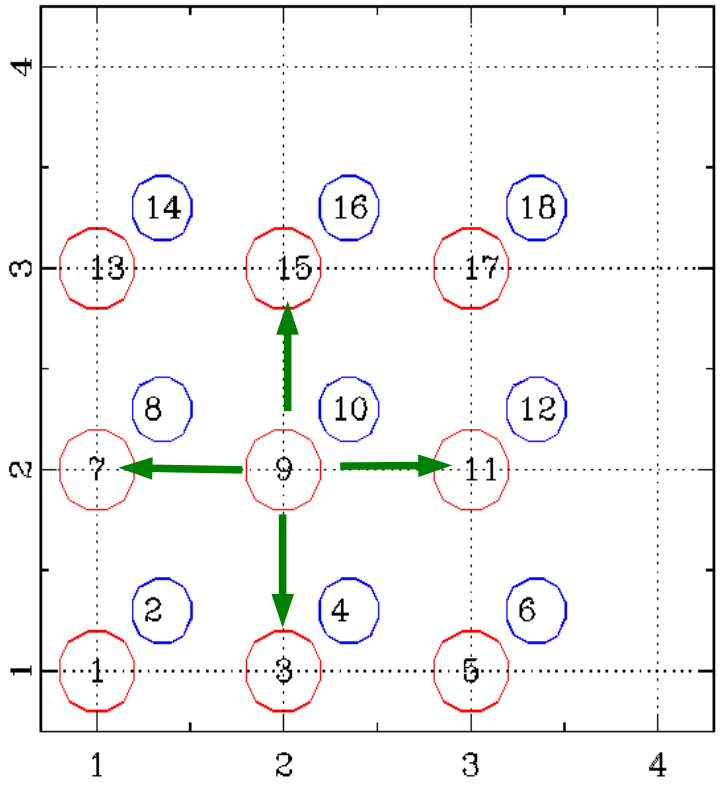
clear tendency to form domains with periodicity **a**



Metropolis et al. J. Chem. Phys. **21**, 1087-1092 (1953)

neigbourhood	which atoms are correlated distance, list of interatomic vectors, ...
correlations	how are atoms related to each other ? chemical — equal atoms <==> different distance — distance between atom pairs angular — bond angle in triplet
modification	how is the crystal structure changed switch two atoms shift individual atoms
Monte Carlo	details of the process number of refinement cycles pseudotemperature kT

Y - axis



X - axis

Neighbors for atom 9

3: site 1 in [0, -1, 0]
7: site 1 in [-1, 0, 0]
11: site 1 in [1, 0, 0]
15: site 1 in [0, 1, 0]

in „chem“ and „mmc“ menus

set vect, 1, 1, 1, 0,-1, 0
set vect, 2, 1, 1, -1, 0, 0
set vect, 3, 1, 1, 1, 0, 0
set vect, 4, 1, 1, 0, 1, 0

This will describe ALL neighbors
of site 1 in any unit cell!
Very fast algorithm to address atoms!

```
# create a structure with randomly distributed atoms...
#
mmc
  set neig,rese                      reset neighborhood
#
  set vec,1, 1,1,  1, 0, 0           Atoms are separated by vector[1,0,0]
                                     Pairs are 1st atoms in any unit cell
  set vec,2, 1,1, -1, 0, 0
  set neig,vec,1,2                   Vector definitions 1,2 are one neighborood
#
  set mode, 1.0, swchem,all          Switch any atom pairs with probability 1.0
#
  set targ,1,corr,cu,void, 0.90 ,0.0,CORR     Correlation energy no. is
                                     chemical bewteen Cu and voids
                                     Target is a C = 0.90
#
  set cyc, 100*n[1]                  No. of cycles is 100 time no. of atoms
  set feed,  5*n[1]
  set temp, 2.0                      Temperature kT = 2.0
  run                                start the calculation
exit
#
```

Binary System with two atom types

Composition 50:50

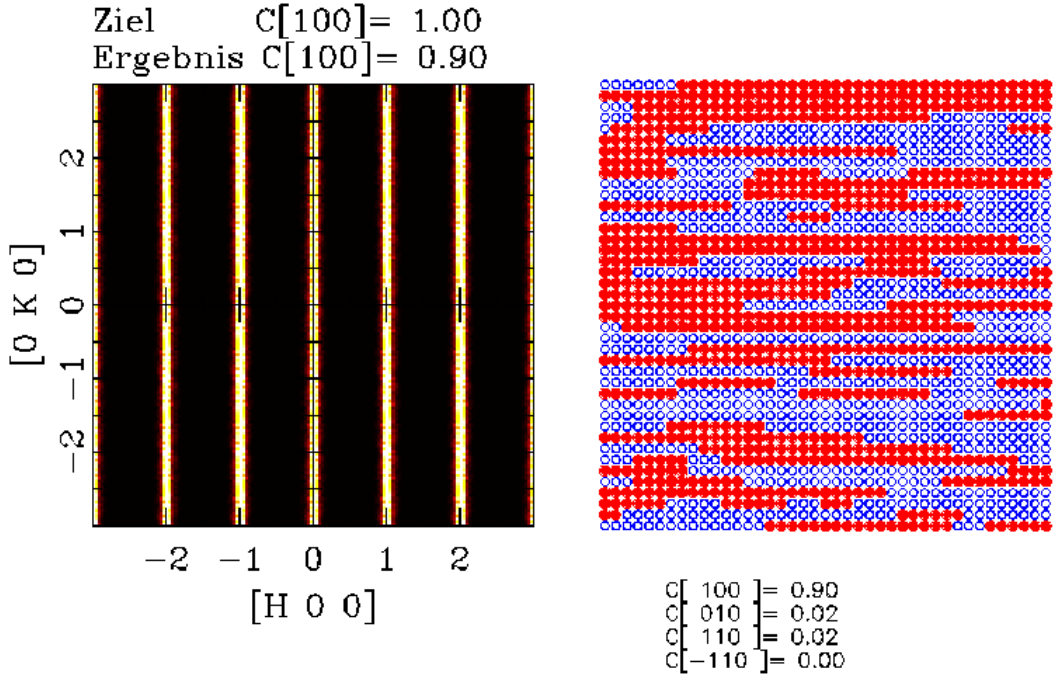
First neighbor correlations only:

Chemical short range order

[1, 0, 0]; [$\bar{1}$, 0, 0]
[0, 1, 0]; [0, $\bar{1}$, 0]
[1, $\bar{1}$, 0]; [$\bar{1}$, 1, 0]
[1, 1, 0]; [$\bar{1}$, 1, 0]

Target:

C [1, 0, 0] = 1.0



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Composition 50:50

First neighbor correlations only:

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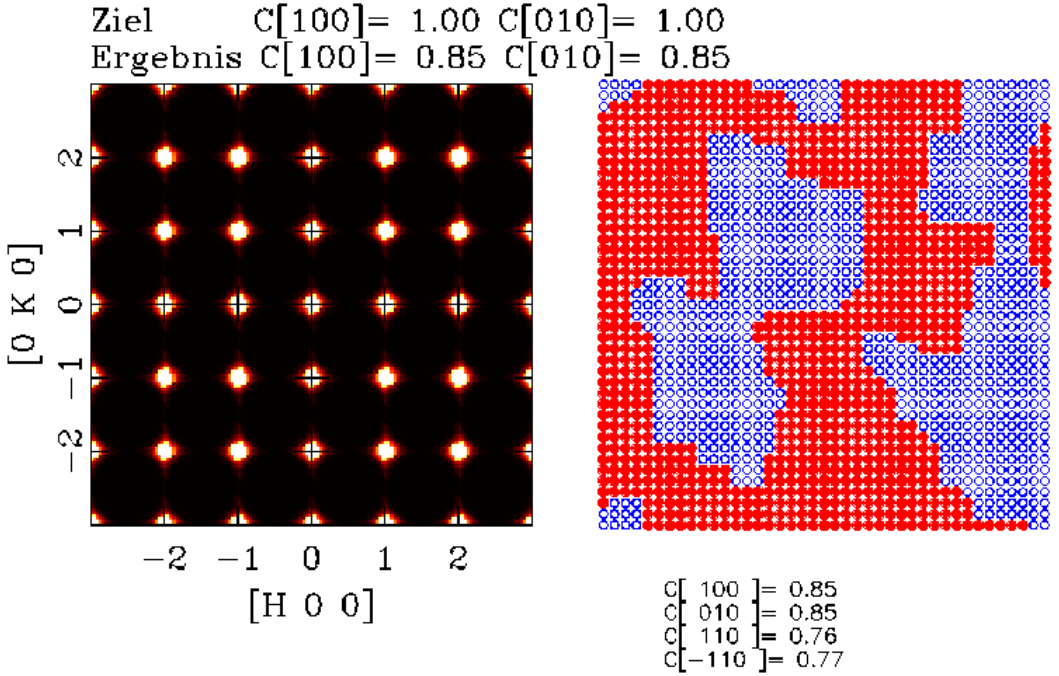
[1, 0, 0]; [$\bar{1}$, 0, 0]
[0, 1, 0]; [0, $\bar{1}$, 0]
[1, $\bar{1}$, 0]; [$\bar{1}$, 1, 0]
[1, 1, 0]; [$\bar{1}$, $\bar{1}$, 0]

Target:

C [1, 0, 0] = 1.0
C [0, 1, 0] = 1.0

Consequence:

C [1, $\bar{1}$, 0] = 1.0
C [1, 1, 0] = 1.0



Binary System with two atom types

Composition 50:50

First neighbor correlations only:

[1, 0, 0]; [$\bar{1}$, 0, 0]
[0, 1, 0]; [0, $\bar{1}$, 0]
[1, $\bar{1}$, 0]; [$\bar{1}$, 1, 0]
[1, 1, 0]; [$\bar{1}$, $\bar{1}$, 0]

Chemical short range order

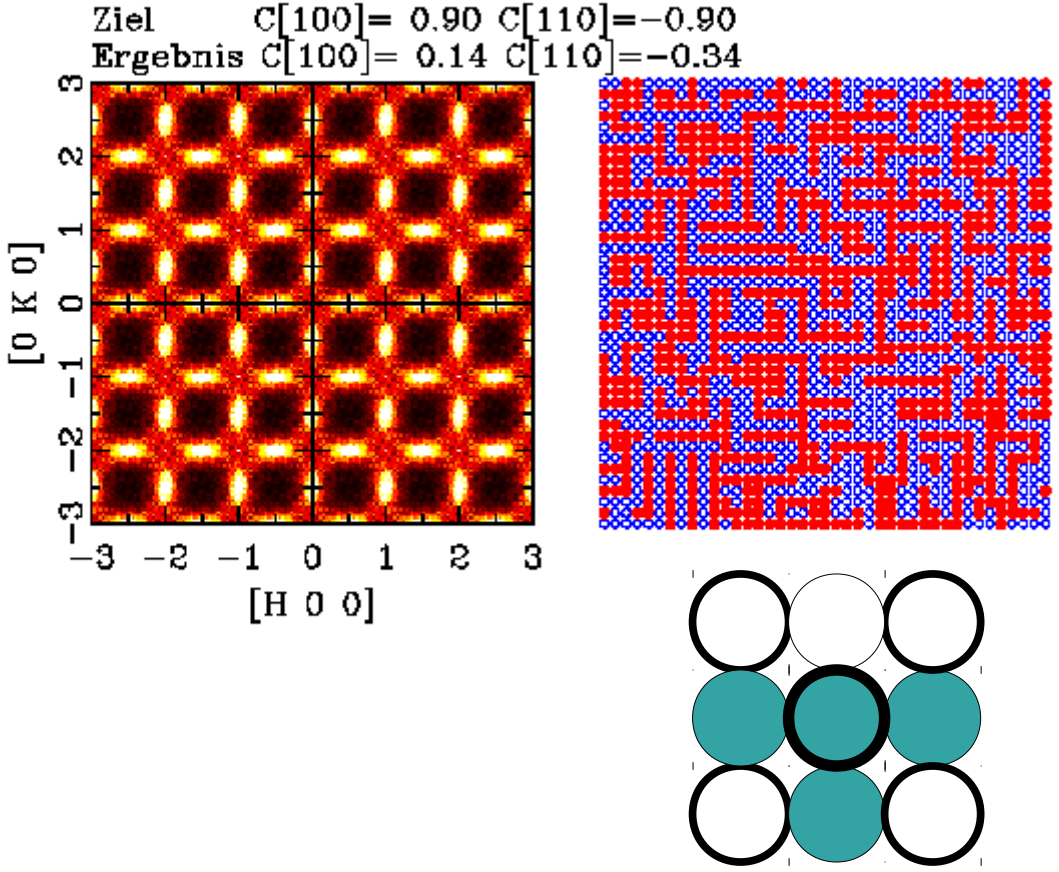
Target:

C [1, 0, 0] = 1.0
C [0, 1, 0] = 1.0
C [1, $\bar{1}$, 0] = -1.0
C [1, 1, 0] = -1.0

Consequence:

C [1, $\bar{1}$, 0] = 0.14
C [1, 1, 0] = -0.34

Contradictory requests!

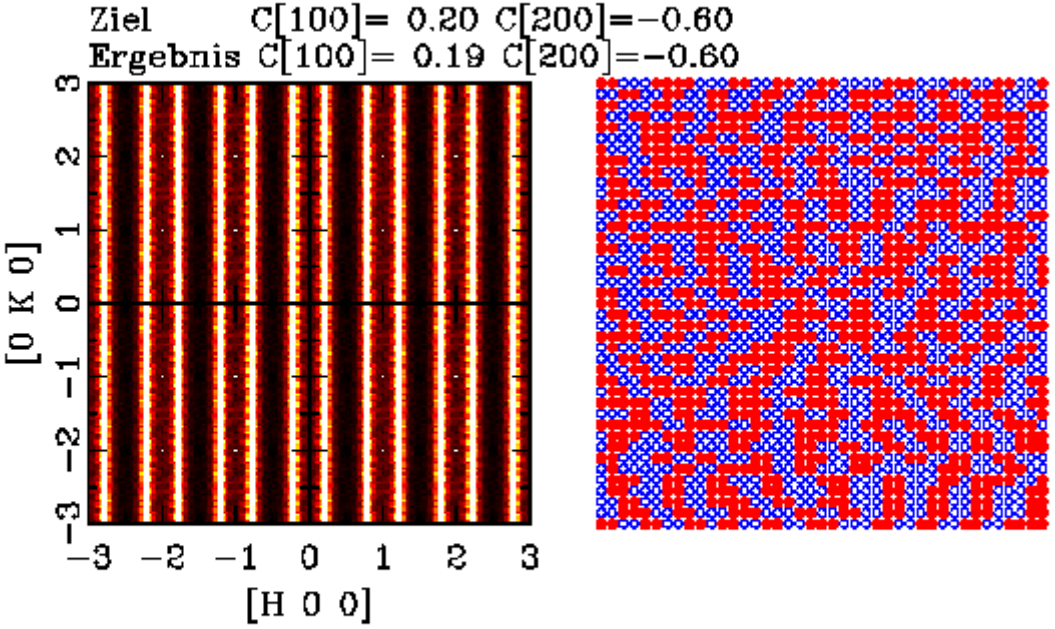


Binary System with two atom types

Composition 50:50

First AND second neighbor
[1, 0, 0]; [$\bar{1}$, 0, 0]
[2, 0, 0]; [$\bar{2}$, 0, 0]

Chemical short range order



Target:
C [1, 0, 0] = 0.2
C [2, 0, 0] = -0.6

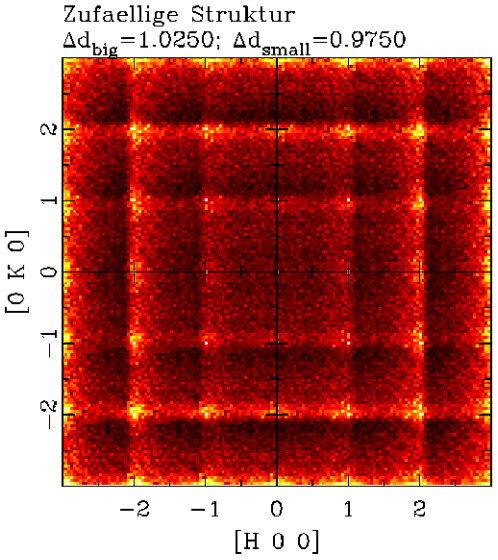
Consequence:
Tendency to form pairs
AA BB AA ...

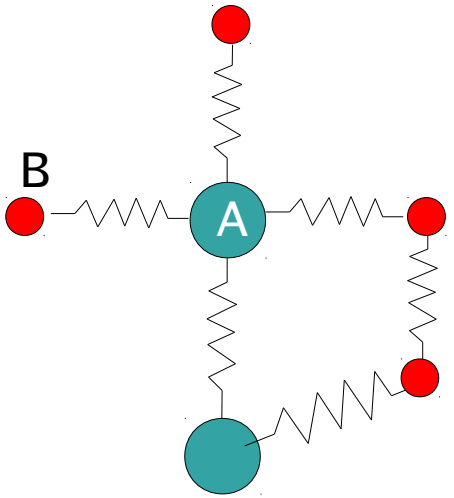
Distance Correlations:

Potential between atom pairs: $U(r) = \frac{A}{r^{12}} - \frac{B}{r^{6}}$

Angular potential: $U(\Theta) = K(\Theta - \Theta_0)^2$

Radii: $r_A > r_B$





[100]

[010]

Form factors $f_A > f_B$

Asymmetrically shaped diffuse scattering
Higher intensity at smaller values of h
“size effect”

Run discus_suite

Change to directory:
Lectures/04.SRO/SRO_1

Use macro: sro.1 with two parameters: <correlation>, <Temperature>

suite> @sro.1.mac 0.8, 5.1
suite> @sro.1.mac -0.7, 5.1

Be creative with the Parameters!

Run discus_suite

Change to directory:
Lectures/04.SRO/SRO_4

Use macro: sro.4.mac with two parameters: <strain>, <Temperature>

suite> @sro.4.mac 0.05, 5.1
suite> @sro.4.mac -0.05, 5.1

Be creative with the Parameters!

Run discus_suite

Change to directory:
Lectures/04.SRO/SRO_3

Use macro: sro.1 with six parameters:
<composition>, <c100>, <c010>, <c110>, <c$\bar{1}$10>, <Temperature>

suite> @sro.3.mac 0.5, 0.4, 0.4, 0.3, 0.3, 1.0
suite> @sro.3.mac 0.5,-0.7, 0.8, -0.6, 0.9, 1.0

Be creative with the Parameters!