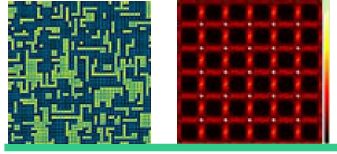
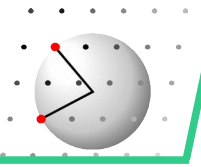


tutorial session VI

domains



domain

(3D) extended modification of the crystal structure

locally changed structure	domains in a strict sense some nm to some µm
local dissolutions	cluster

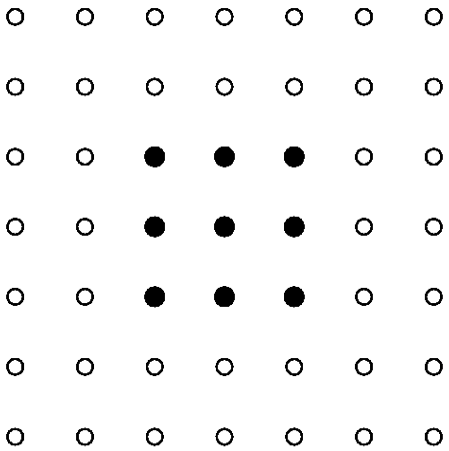
aspects needed to describe a domain

orientation relationship host <==> guest	(ir)regular intergrowth $lattice_{host}$ <==> $lattice_{guest}$
interface host <==> guest	smooth interface rough, irregular interface
distribution of domains	(irr)regular distribution

origin

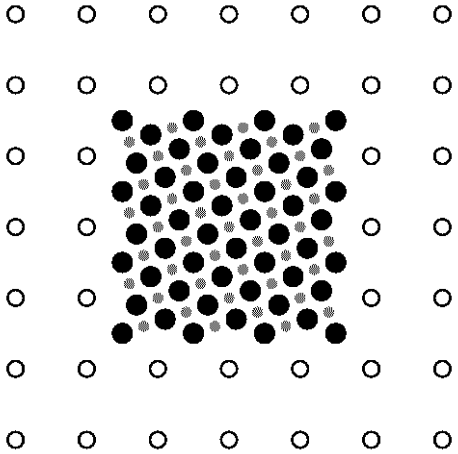
very often in connection with phase transitions
indirectly in relation to host/guest structures and intercalated structures

Introductory examples



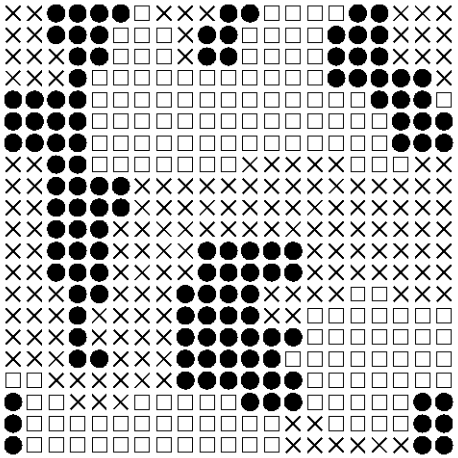
simple domain
identical lattice
smooth interface

if randomly distributed:
diffuse maxima at
common Bragg reflections



simple domain
different structure
smooth interface

if randomly distributed:
diffuse maxima at
individual Bragg reflections



simple domain
different structure
uneven interface

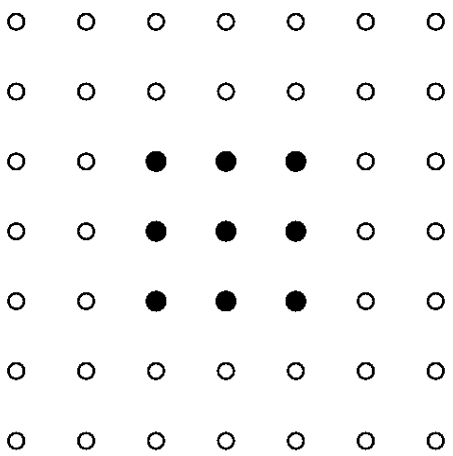
diffuse maxima at
individual Bragg reflections

Exercise 1

Run discus_suite
Switch to directory:
Lectures/06.domain/CUBE

Use Macro dom.cube.mac

suite > @dom.cube.mac



Use

jmol with file cube.cif

As well

```
read                                                # switch to read menu
cell dom.host.cube.cell,7,7,1                       # read an asymmetric unit expand
#
domain                                              # switch to domain level
  rese                                              # reset everything
  mode   pseudo                                     # Interpret pseudo atoms
  input  dom.cube.pseudo                            # List of domain origins
  assign char,si,cube                               # interpret "SI" as a cube shaped
  assign fuzzy,si,1.5                               # define distance to host atoms
  assign cont, si,dom.guest.cube.stru               # domain structure is in this file
  assign shape ,si,1,  1. , 0. , 0. ,  0.           # Define a cube shaped domain
  assign shape ,si,2,  0. , 1. , 0. ,  0.           # that is +- 1 unit cells large
  assign shape ,si,3,  0. , 0. , 1. ,  0.           #
  assign orient,si,1,  1. , 0. , 0. ,  0.           # Domain content shall be rotated
  assign orient,si,2,  0. , 1. , 0. ,  0.           # by this matrix (here unit matrix)
  assign orient,si,3,  0. , 0. , 1. ,  0.           #
  set    distance, all, 2.55                        # Define distance to internal
  set    distance, new, 2.71                        # boundary for old and new atoms
  show
  run
exit
```

```
title Domain list for simple domains
spcgr  P4
cell   2.50, 2.50, 2.50, 90.00, 90.00, 90.00
atom
SI   0.00000  0.00000  0.00000   0.05
```

The domain list is a simple DISCUS structure file

Here one pseudo atom at 0,0,0

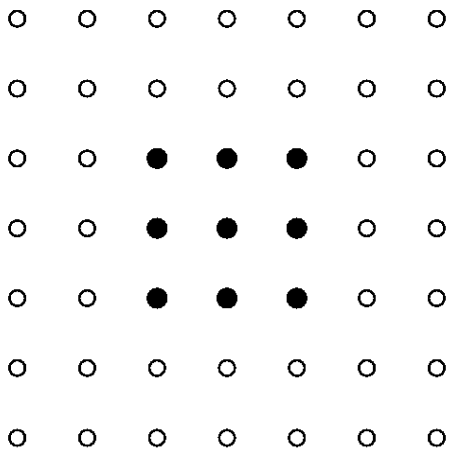
Exercise 2

Run discus_suite

Switch to directory:
Lectures/06.domain/CUBE

Use Macro dom.cube.mac

suite > @dom.cube.mac



Edit file dom.cube.pseudo
Change the position of the SI atom,
Add new SI atoms...

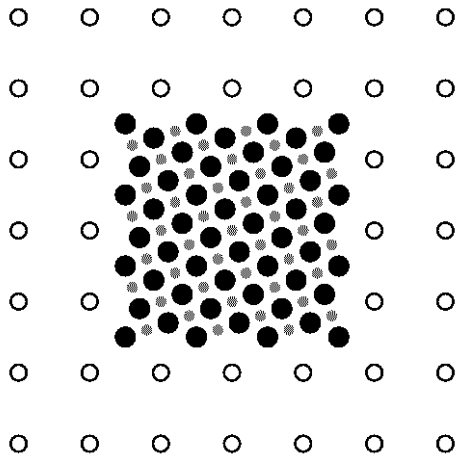
Use

jmol with file cube.cif

as well

Run discus_suite

Switch to directory:
Lectures/06.domain/CUBE



Use Macro dom.tilt.mac

suite > @dom.tilt.mac

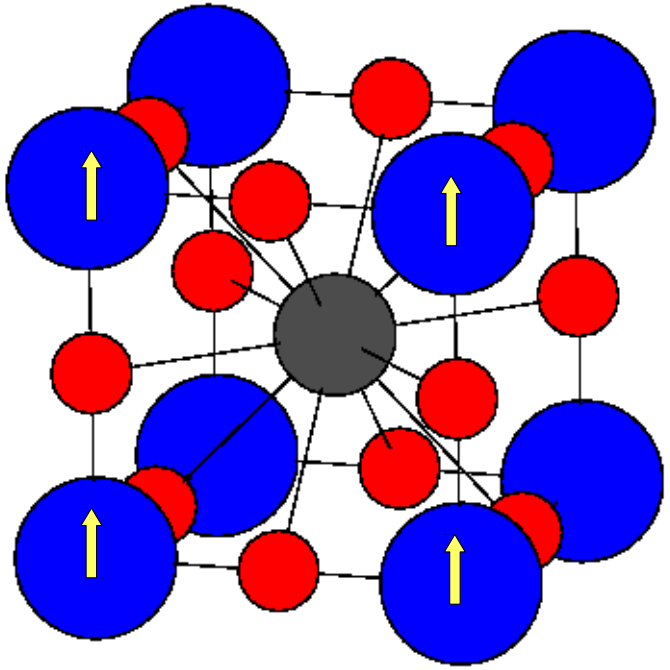
Edit file dom.tilt.mac
Lines 46 to 48 contain a rotation matrix

Use

jmol with file tilt.cif

as well

Example: Perovskite



high temperature phase

cubic Pm3m

Ti **0,0,0** **octahedron site**

Sr **½, ½, ½**

O **½,0,0**

low temperature phase (simplified)

tetragonal P4mm

c/a ≠ 1

shift of Ti along [001]

in Pm3m equivalent: [100] [010] [001]

independent nucleation three different possible orientations

relaxation within one unit cell equal relaxation in neighboring cells

simulation of the disordered low temperature structure

A) random selection of individual unit cells ==> introduce a local distortion

relax neighboring cells (in random sequence)
until whole crystal has been distorted

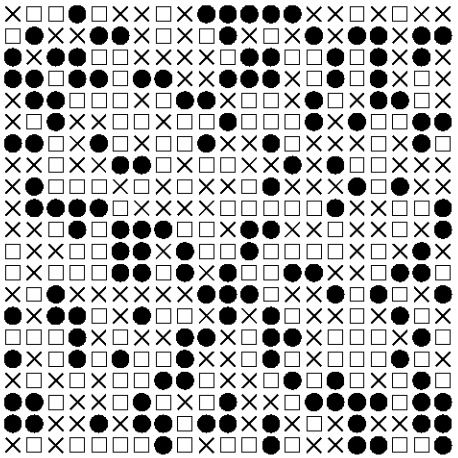
extended book keeping and search for unit cells that are distorted already!

B) 'detour' via dummy-atoms (dummy-domains)

1. cubic primitive crystal with three different atoms A,B,C at equal amounts
2. sort atoms A,B,C with positive correlation
3. relax distances A-A, B-B, C-C
4. replace atoms A by unit cell distorted along [100]
   replace atoms B by unit cell distorted along [010]
   replace atoms C by unit cell distorted along [001]

B) 'detour' via dummy-atoms (dummy-domains)

1. cubic primitive crystal with three atoms A,B,C in equal amounts



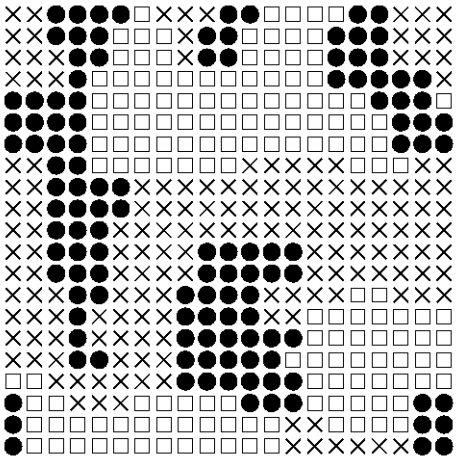
atom A represents a unit cell
that is distorted along [100]
correpondingly for B and C

Distance between atoms: lattice constant a
atom position: 0,0,0

2. sort atoms A,B,C with positive correlations

Neighbors along: <100>

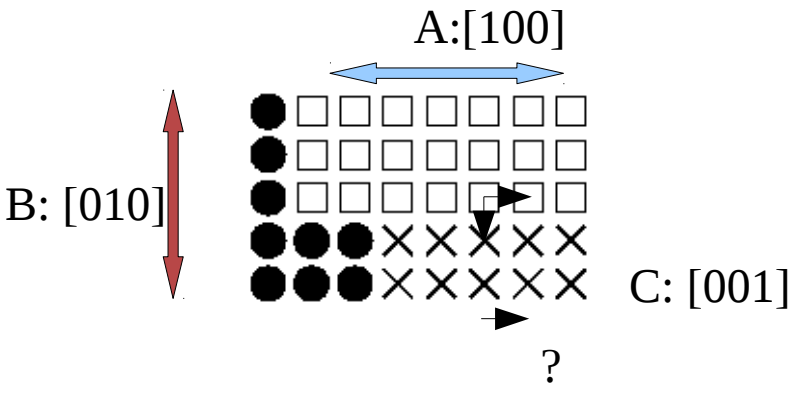
pairs: A-B, A-C, B-C
each with correlation > 0



Crystal, build up of three different 'atoms',
all at ideal positions, no distortions

B) 'detour' via dummy atoms (dummy domains)

3. local distortions

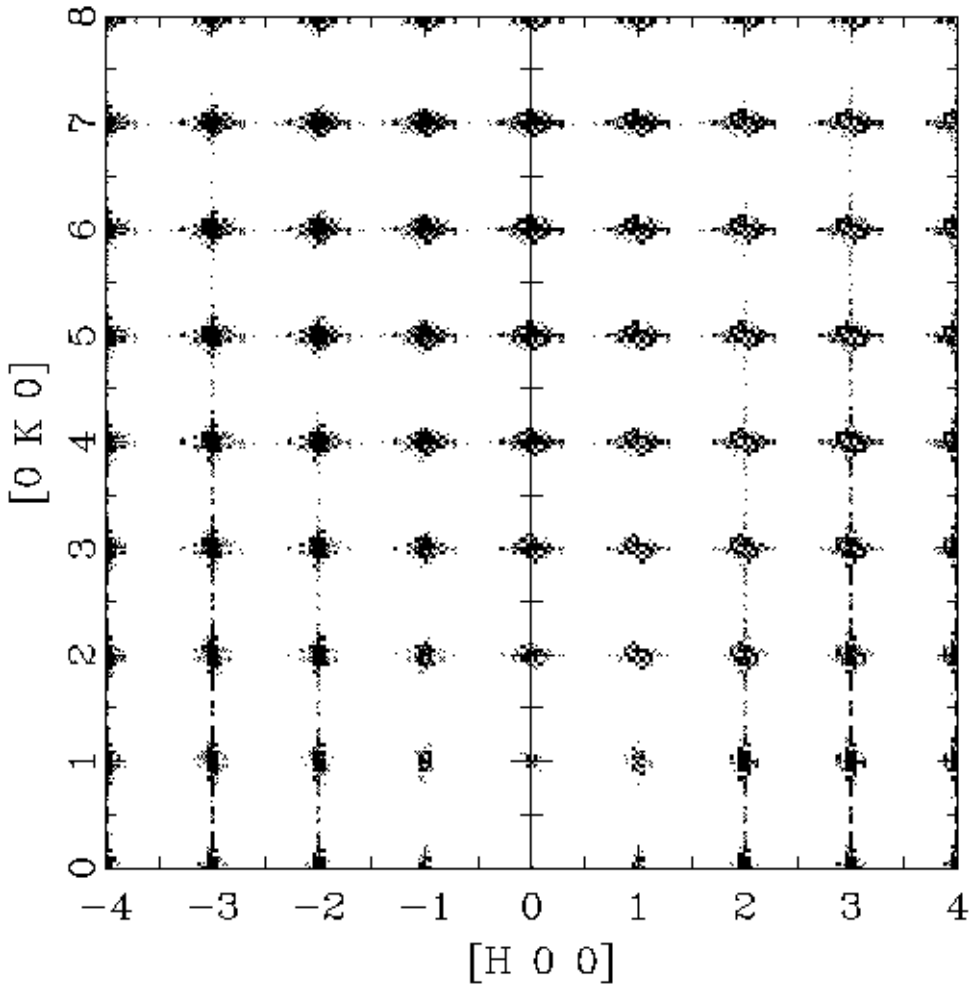


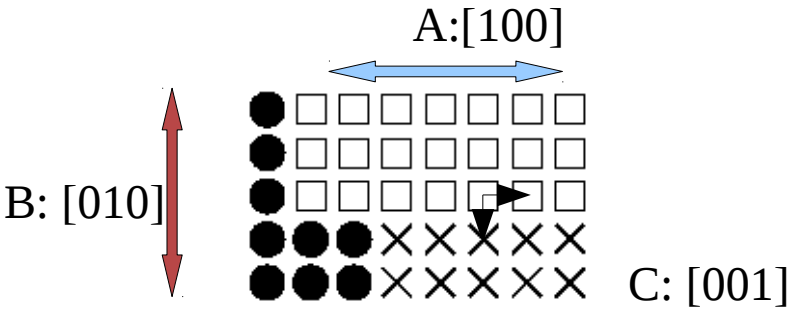
pair A-A: distanc along	[100] is a_0*k [010] is a_0/k [001] is a_0/k	with k ~ 1.0025
pair A-X: distance along	[100] is a_0 [010] is a_0 [001] is a_0	distortion of A along [100] induces shift of /C along [100] If interface is long, dislocations will occur
angle A-A-A	90°	

Example: Perovskite

diffraction pattern of the relaxed structure

all 'atoms' are identical!





diffuse maxima at Bragg positions

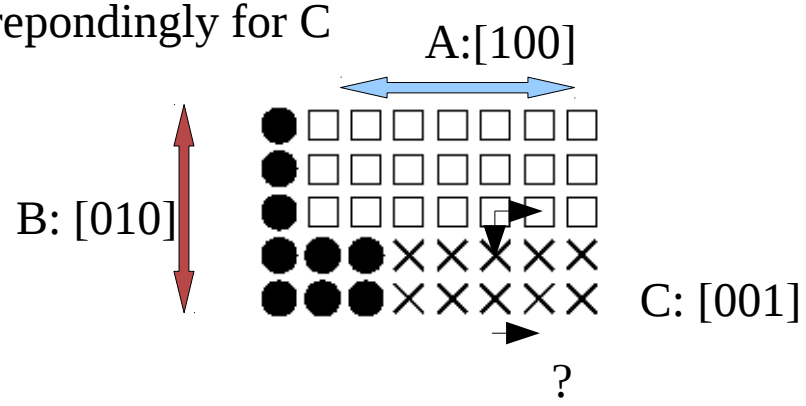
extended domains of locally equal atoms

weak diffuse streaks

shift of the domains

B) 'detour' via dummy atoms (dummy domains)

4. replace atoms A by a unit cell that is distorted along [100]
correspondingly replace B by a unit cell that is distorted along [010]
correpondingly for C



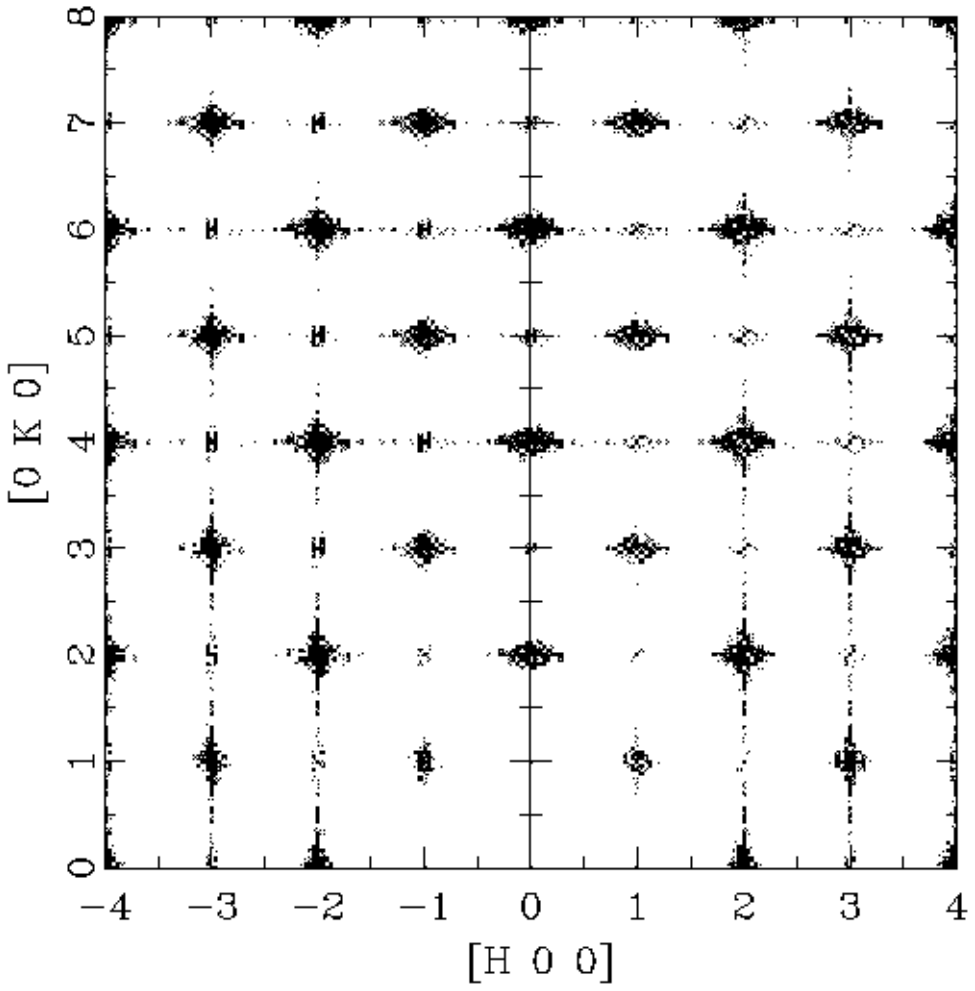
metric remains cubic

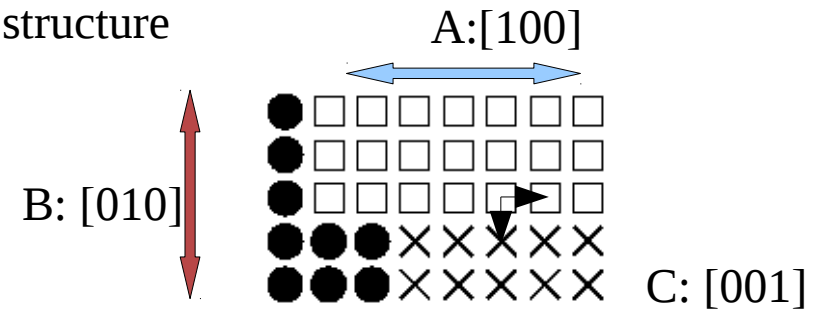
transform atoms within a [100] domain by:

$$\begin{pmatrix} k & 0 & 0 \\ 0 & 1/k & 0 \\ 0 & 0 & 1/k \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

in addition, relative shift of atoms along ±[100]

diffraction pattern of the relaxed and replaced structure





diffuse maxima at Bragg positions

extended domains that consist of unit cells, locally distorted along the same direction

$I_{h+k+l = 2n} > I_{h+k+l = 2n+1}$

weak diffuse streaks

shift of domains

Run discus_suite

Switch to directory:
Lectures/06.domain/Perovskite

Use Macro dom.perov.mac

suite > @dom.perov.mac

The macro takes you through the steps
Plots follow at the end