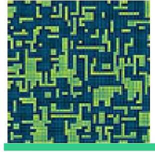
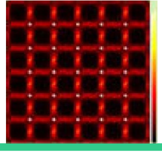
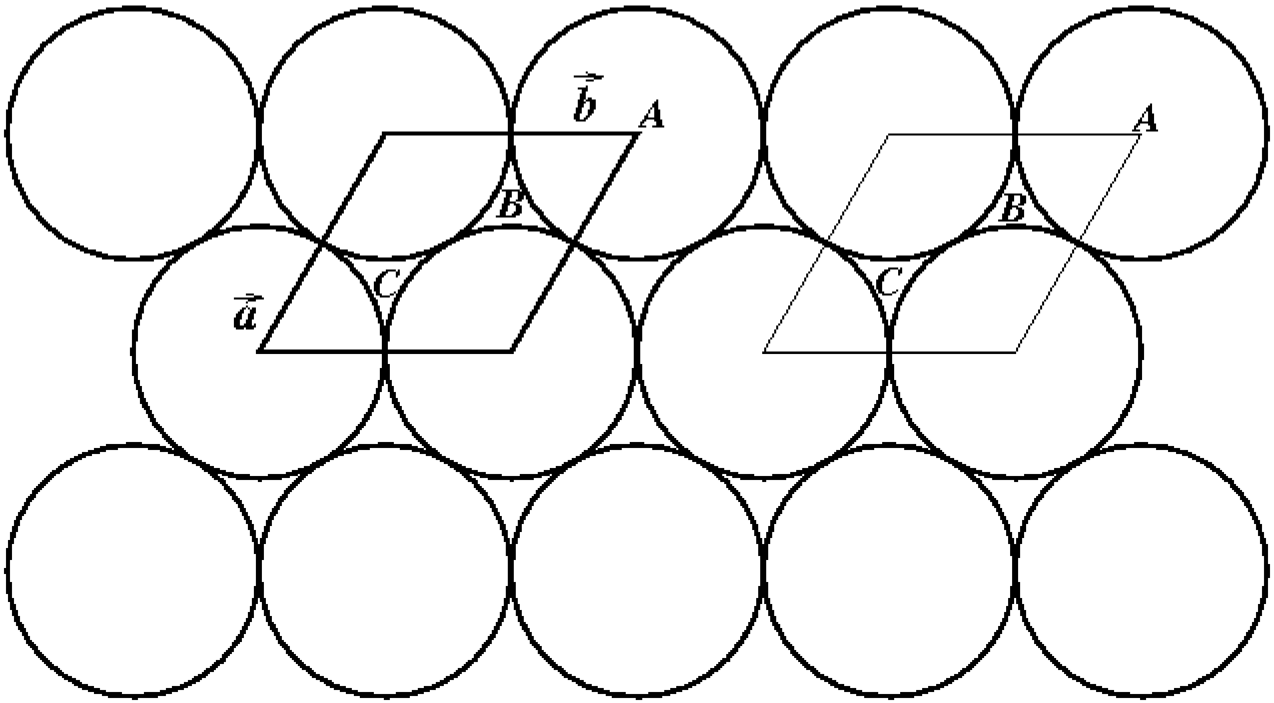
 

tutorial session V

stacking faults

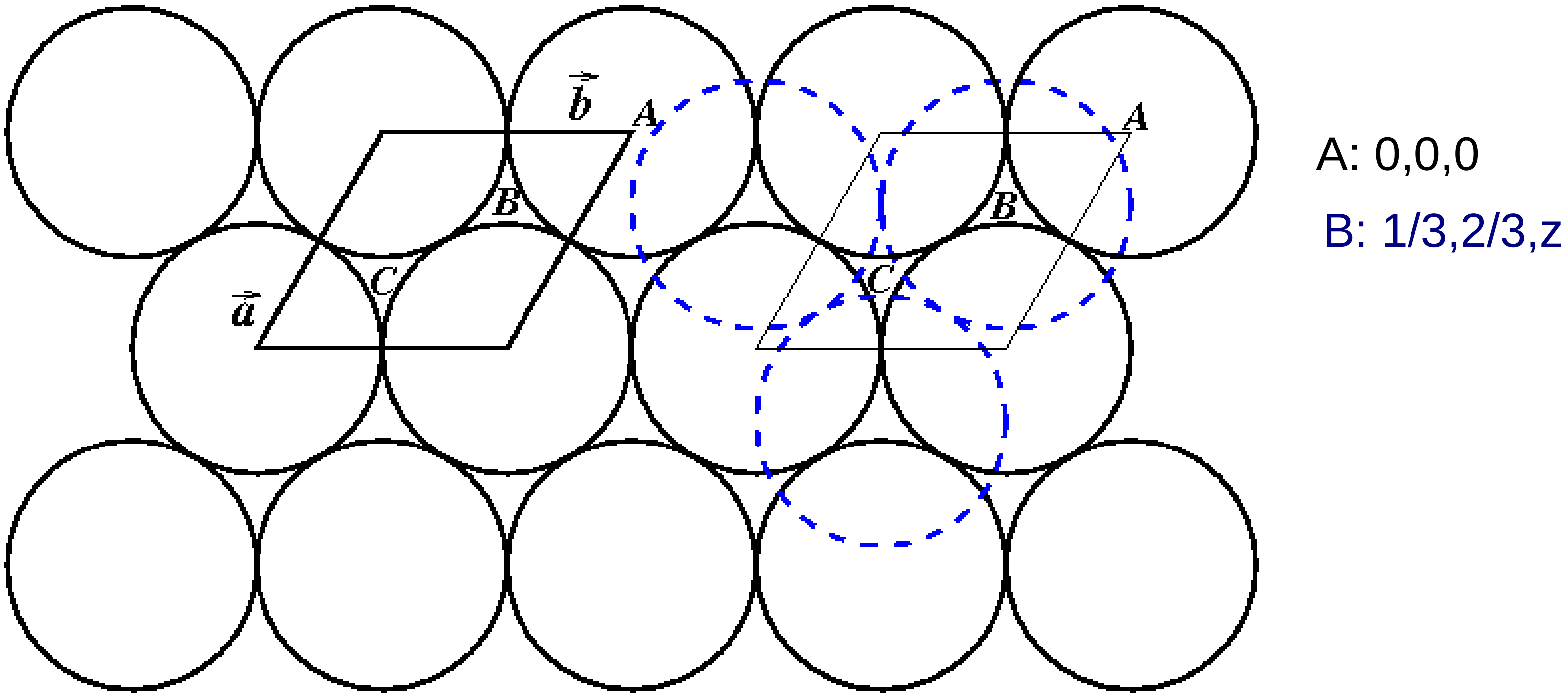
close packed spheres in 2D



A: 0,0,0

position of atoms relative to a hexagonal unit cell

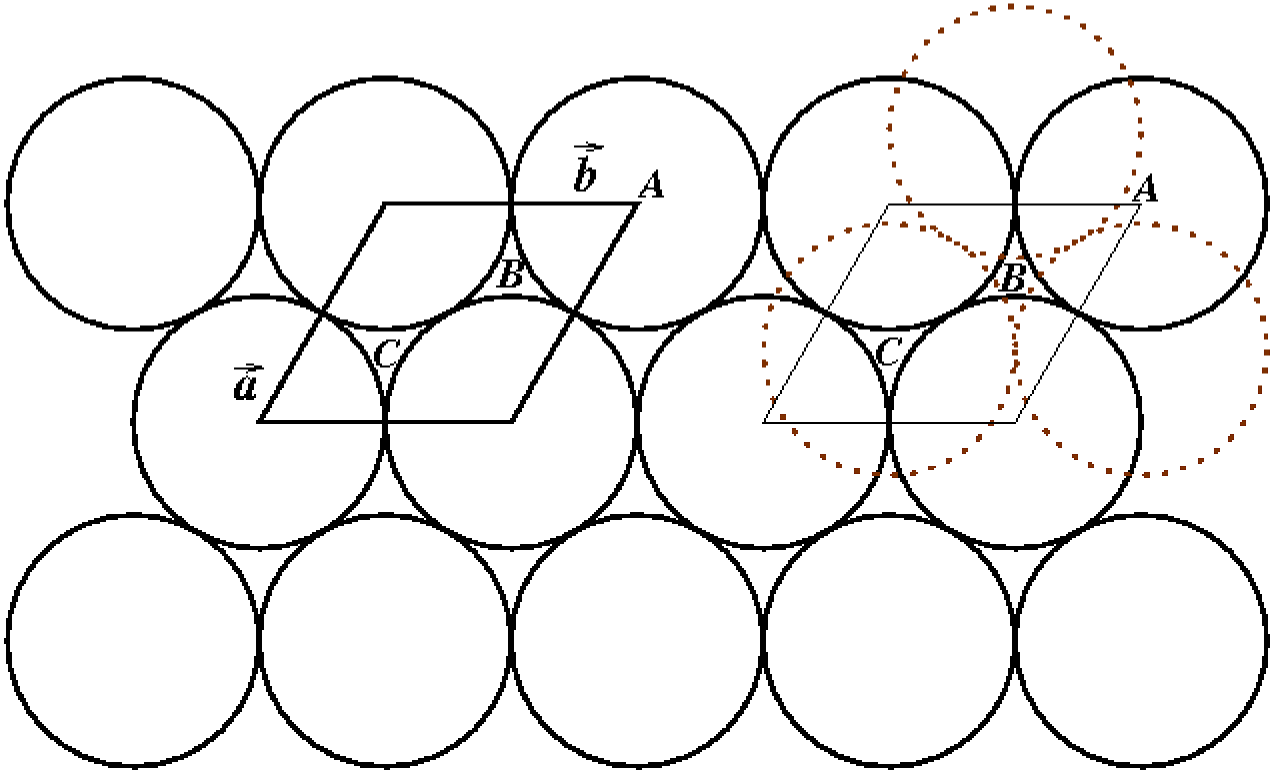
close packed spheres



position of atoms in two adjacent layers A B

if repeated periodically ABABAB... hexagonal closest packing

close packed spheres



A: 0,0,0

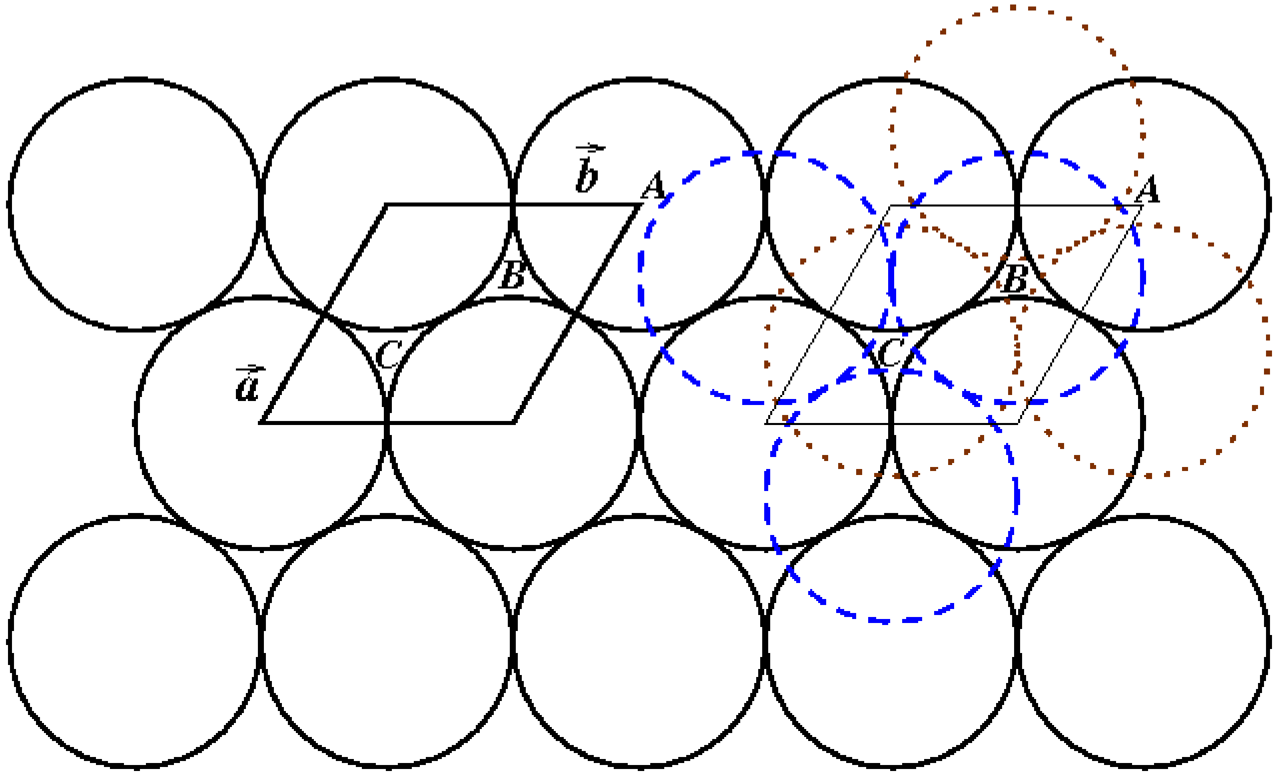
C: 2/3,1/3,-z

Position of atoms in two adjacent layers A C

if repeated periodically ACACAC... hexagonal close packing

ideal hexagonal close pacing $c/a = \sqrt{8/3}$

close packed spheres



A: 0,0,0

B: 1/3,2/3,z

C: 2/3,1/3,-z

atom position in three adjacent layers

if repetaed periodically ABCABC... closed packed

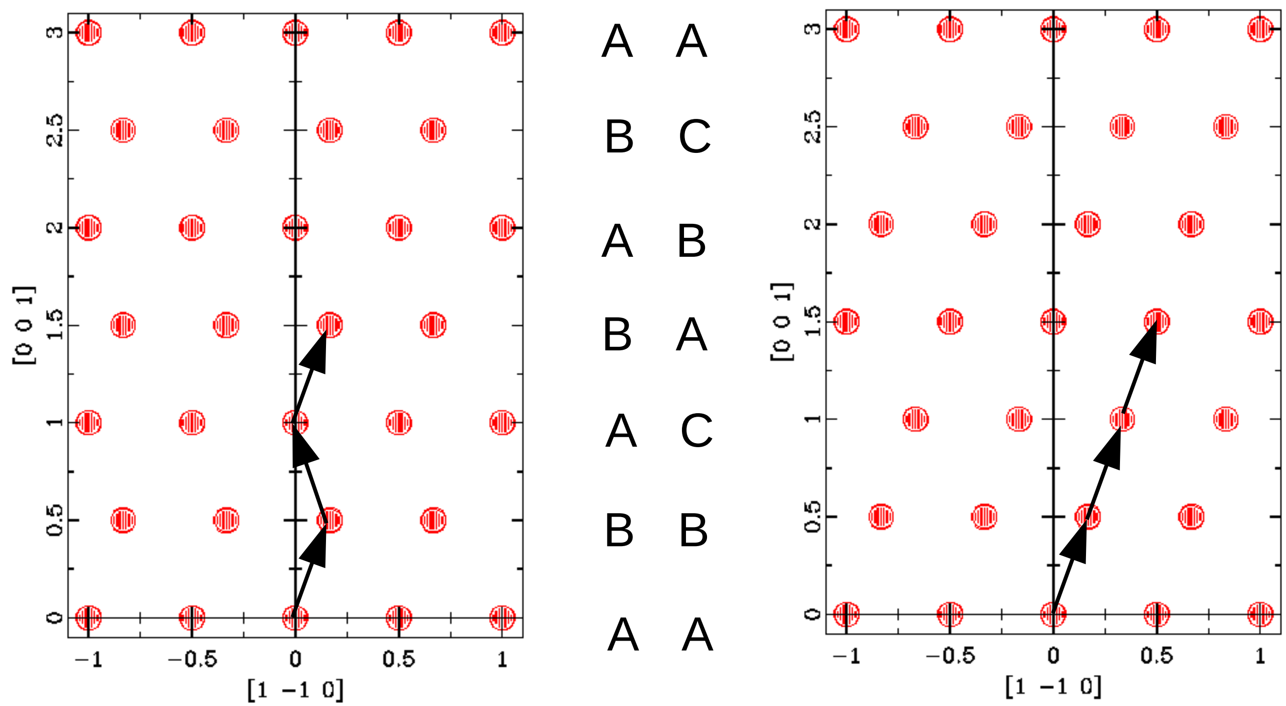
closed packed layer corresponds to **each** of the {111} layers !

layer normal to [110]

1/3 -1/3 1/2

-1/3 1/3 1/2

1/3 -1/3 1/2



1/3 -1/3 1/2

1/3 -1/3 1/2

1/3 -1/3 1/2

identical sequence of any two adjacent layers
except for a possible mirror image at (1-10)

all distances from a given atom to all its neighbors remain identical

almost all bond angles identical

high probability of stacking faults

Reciprocal space of a single layer

basic assumption:

each layer is periodic in 2-dimensional: perfectly flat, infinitely extended

the Fouriertransform of a **single** layer is given by

$$F(\vec{h}) = \sum_{atoms} b\, e^{2\pi i\, \vec{h}\, \vec{r}}$$

$$F(hkl) = \sum_{atoms} b\, e^{2\pi i\,(hx + ky + lz)}$$

z= 0 for all atoms

$$F(hkl) = \sum_{atoms} b\, e^{2\pi i\,(hx + ky)}$$

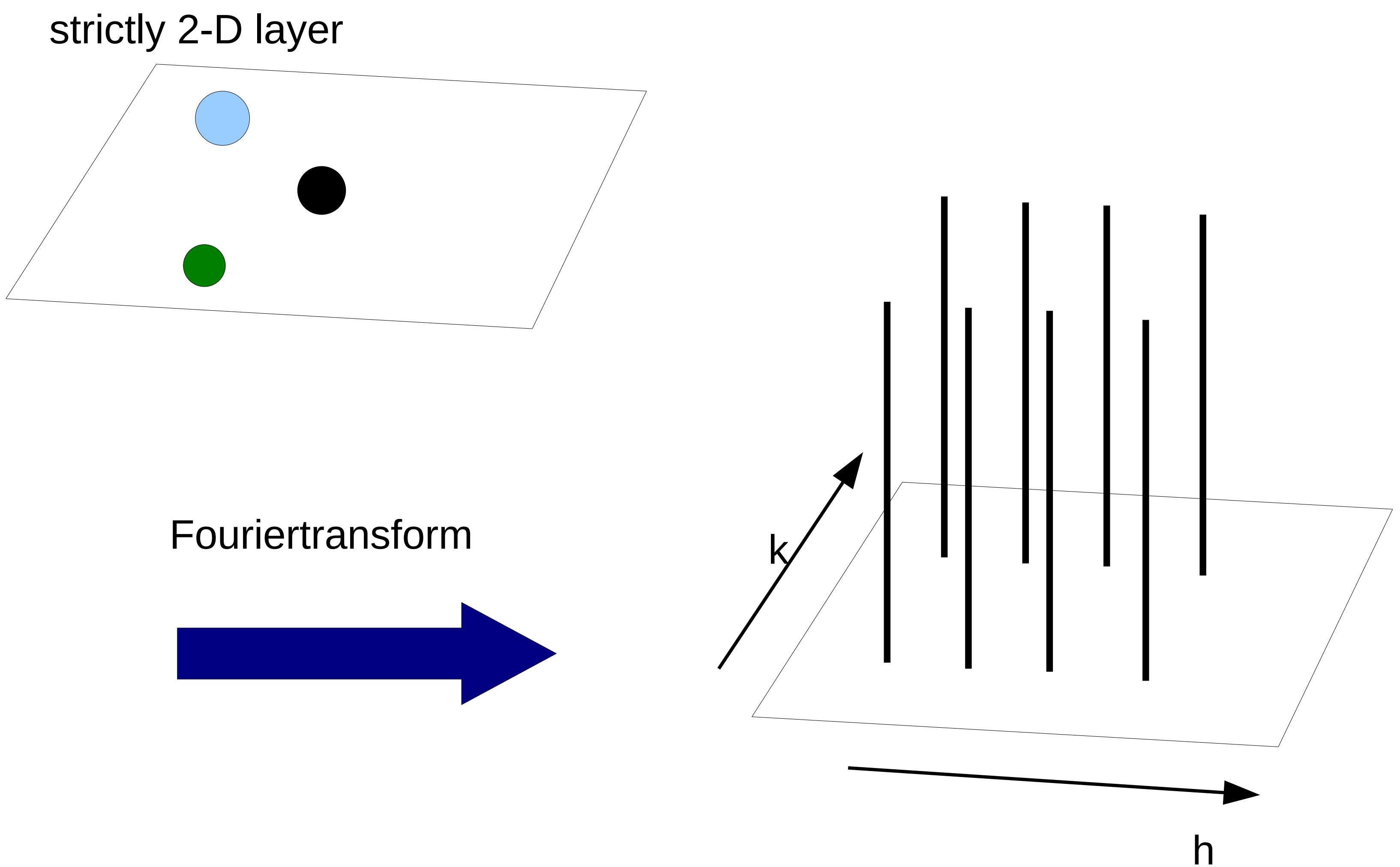
→ F(hkl) independent of l

periodic in x and y → F(hkl) ≠ 0 only for h,k integer

→ Fourier transform consists of rods parallel l at h,k integer

$$\vec{c}^{\,*} = \frac{\vec{a} \times \vec{b}}{V}$$

→ rods are normal to the layer


strictly 2-D layer
Fouriertransform
k
h

1. crystal consist of identical layers shifted with respect to each other :

crystal = origins of individual layers ⊗ atoms with a single layer

⊗ = convolution

Fouriertransform:

$\mathscr{F}$ (origins) * $\mathscr{F}$ (individual layer)

rods parallel l at h,k integer

generally a continuous
function in reciprocal space

also rods of (diffuse) intensity in reciprocal space
intensity distribution along the rods depend on the
distribution of the origins

example

comparison hexagonal / cubic closed packing

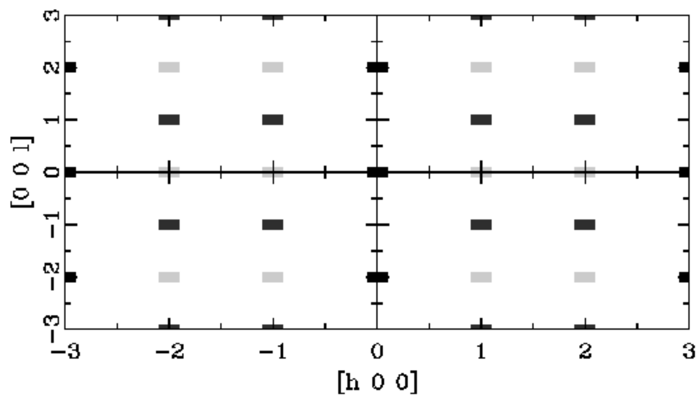
H0L layer in hexagonal metric

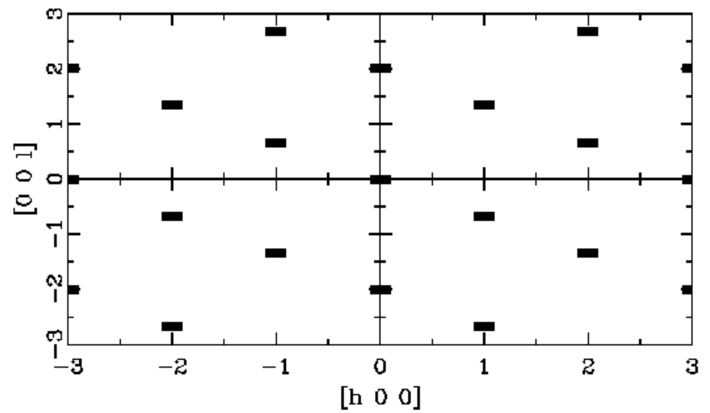
Extinction rules

00l l=2n
hkl l=2n or
h-k = 3n+1 or
h-k = 3n-2

hkl h,k,l = ggg or uuu

Reflections at l = n * 2/3

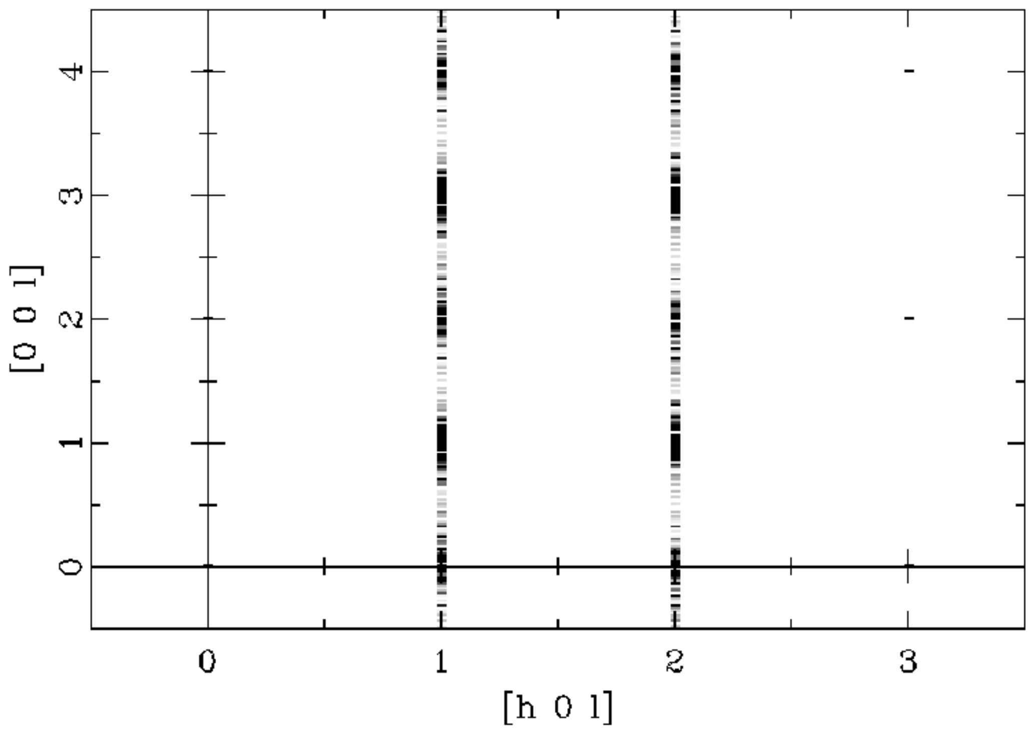




example

Closed backed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



H0L layer
metric: hexagonal
reciprocal lattice

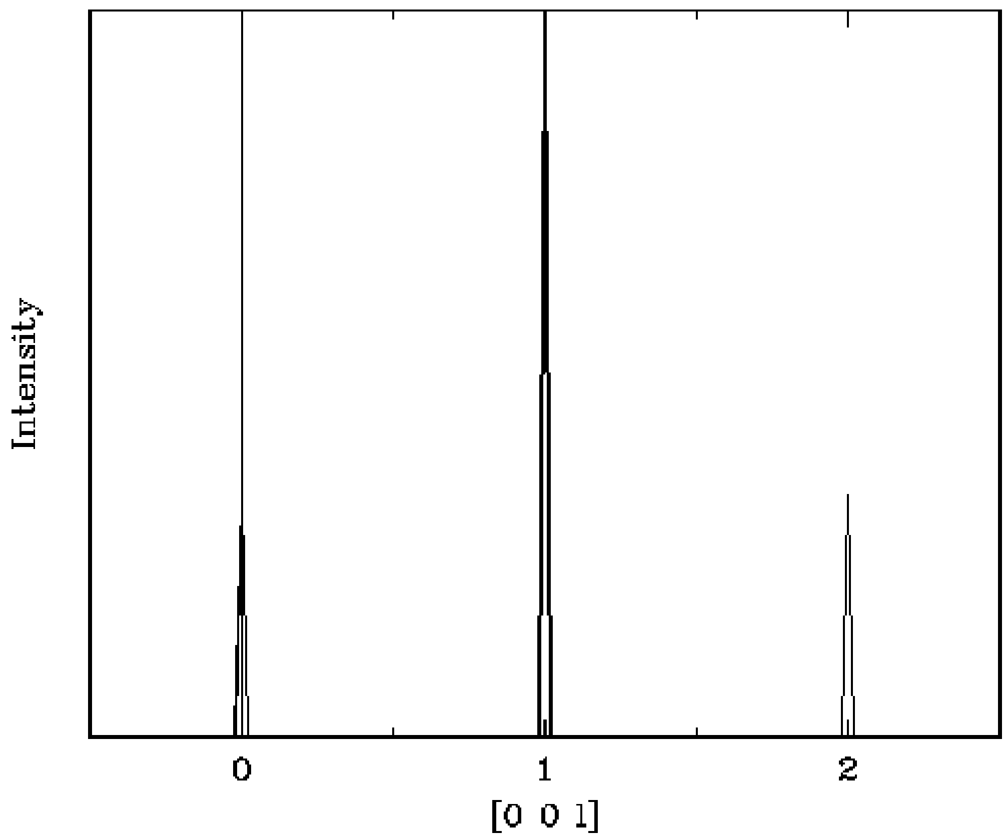
diffuse rods at h ≠ 3n

preferred: ABABAB..

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



H0L layer
metric: hexagonal
reciprocal lattice

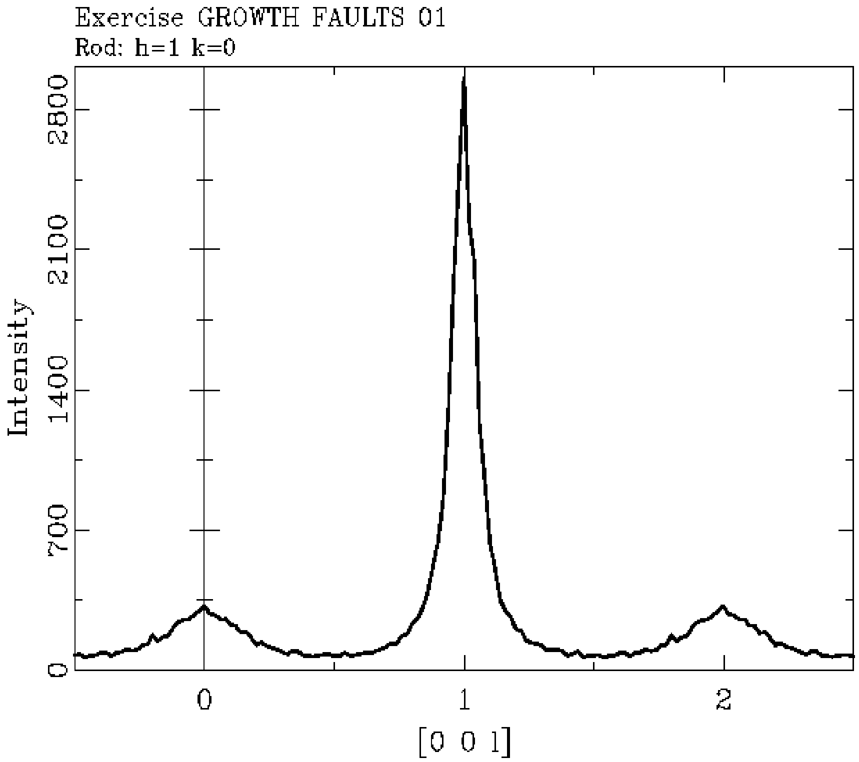
diffuse rods at h ≠ 3n

perfect ABAB.. sequence

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod
Metric: hexagonal
reciprocal lattice

diffuse rods at h ≠ 3n

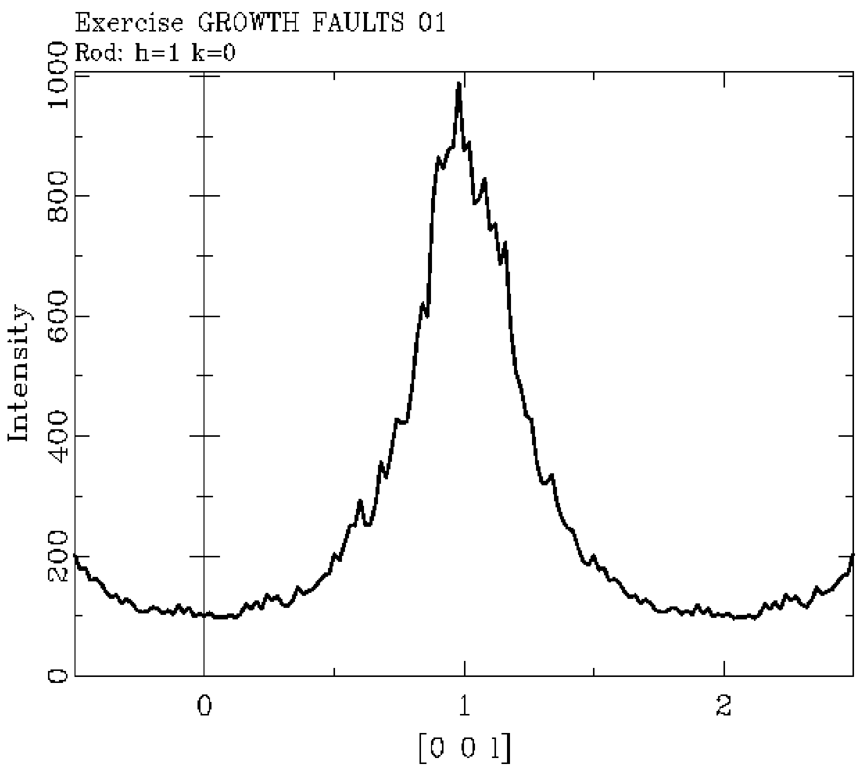
ABAB.. sequence,
25% stacking fault-probability

A B 0.75
A C 0.25

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod
Metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

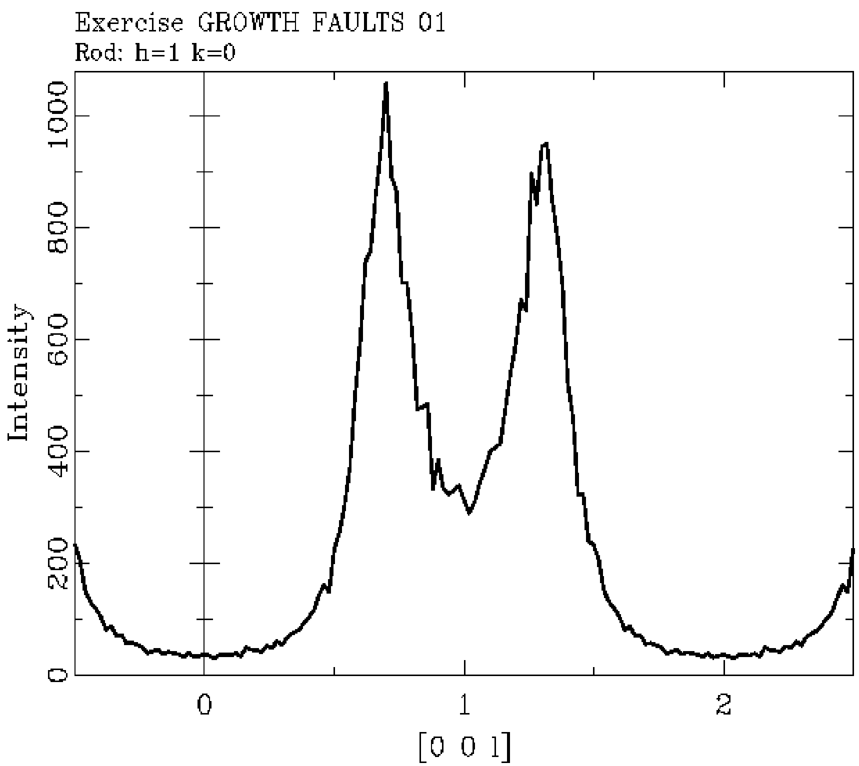
ABAB.. sequence,
50% stacking fault probability

A B 0.50
A C 0.50

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod
Metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

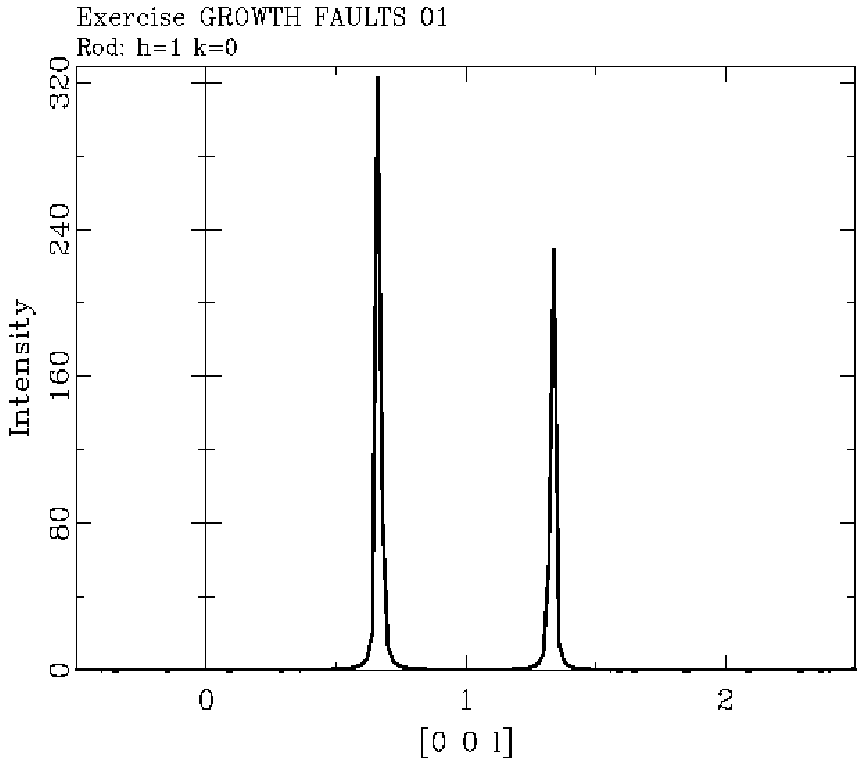
ABAB.. sequence,
75% stacking fault probability

A B 0.25
A C 0.75

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod
Metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

ABAB.. sequence,
100% stacking fault probabiity

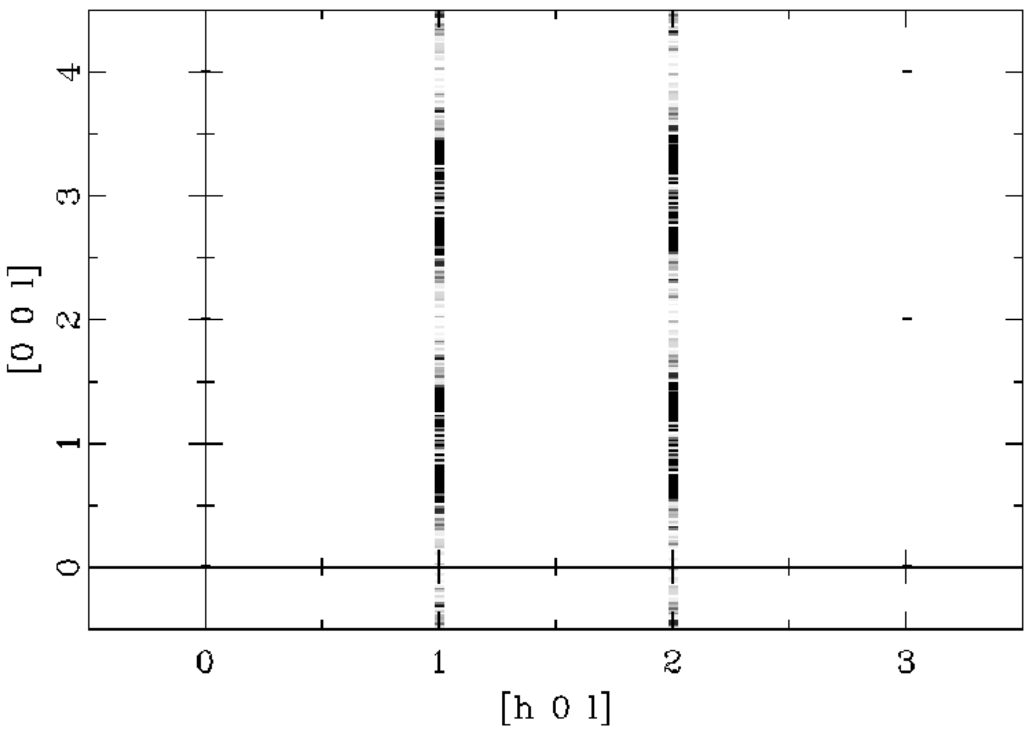
A B 0.00
A C 1.00

Single twinned crystal

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod
Metric: hexagonal
reciprocal lattice

diffuse rods at h ≠ 3n

preferred ABCABC..

layer types A,B,C, ...

atom positions within each layer type dependent on layer sequence ?

vectors from layer to layer

$\vec{ab}, \vec{ac}, \vec{bc}, \vec{ba}, \vec{ca}, \vec{cb}, \ldots$

probabilities for any pair:

A..A, A..B, A..C, B..A, ...:

extend of the interaction

type of layer n is determined by
n-1
n-1, n-2,
n-1, n-2, n-3
...

extend of the layers

across the whole crystal

only a partial layer within the crystal limited by dislocations

all faulted layers parallel to each other ?

Stack of identical layer types A,B,C, ... no diffuse scattering at rod 00L

Stack of different layer types A’,B’,C’, ... also diffuse scattering at rod 00L
Stack of different d-spacings

vectors from layer to layer $\frac{1}{3}\vec{a}$ No diffuse scattering at rod 30L

vectors from layer to layer $u\vec{a}+v\vec{b}+w\vec{c}$

No diffuse scattering at rods where

$uh+vk+wl = 0$