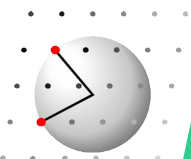


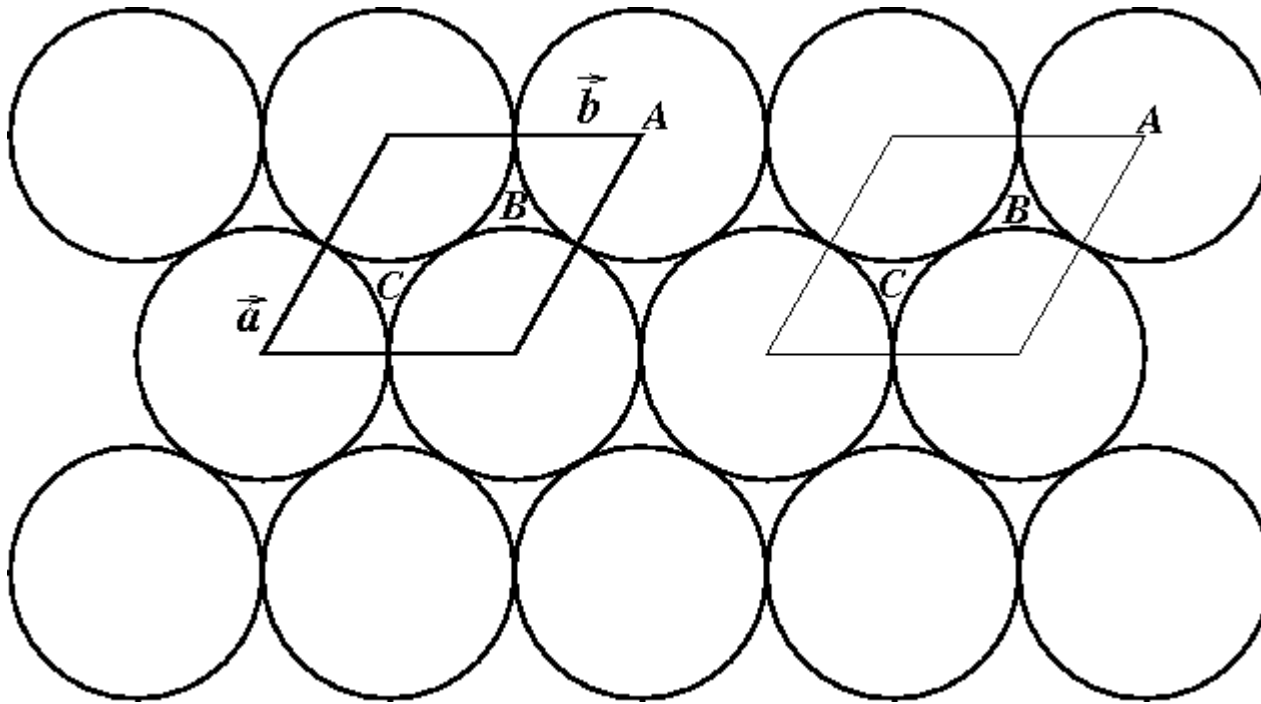


tutorial session V

stacking faults



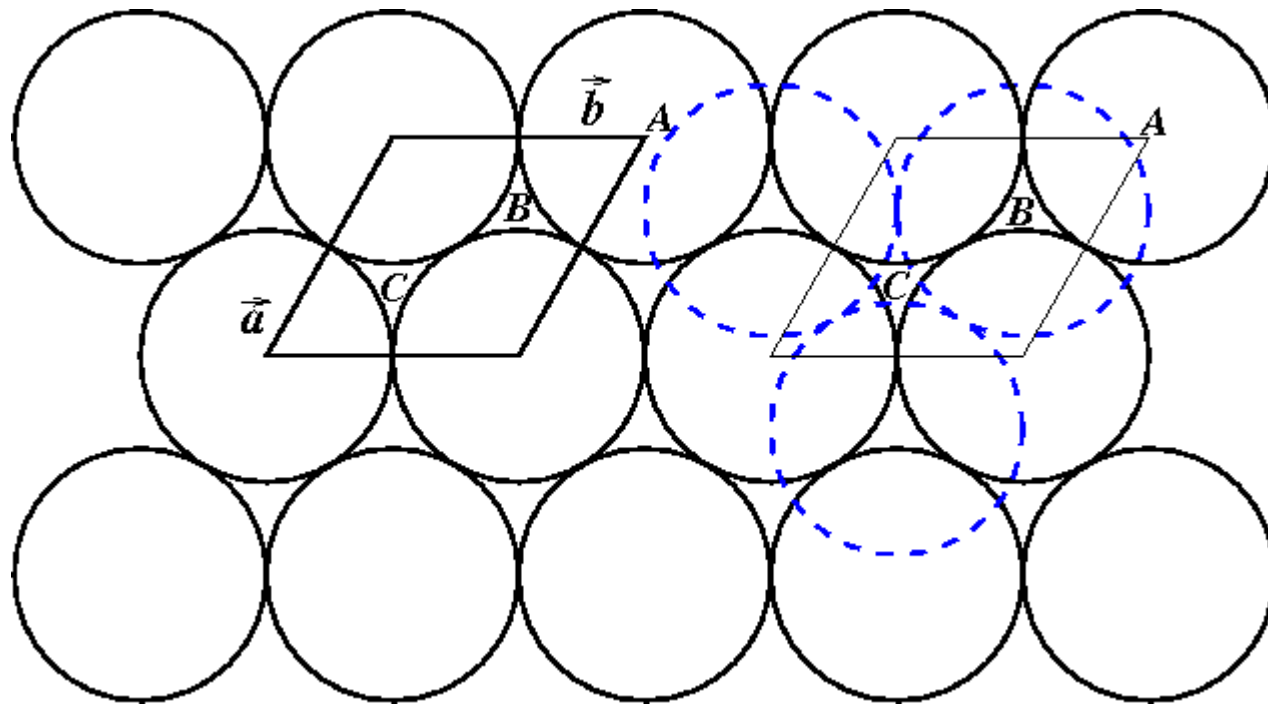
close packed spheres in 2D



A: 0,0,0

position of atoms relative to a hexagonal unit cell

close packed spheres



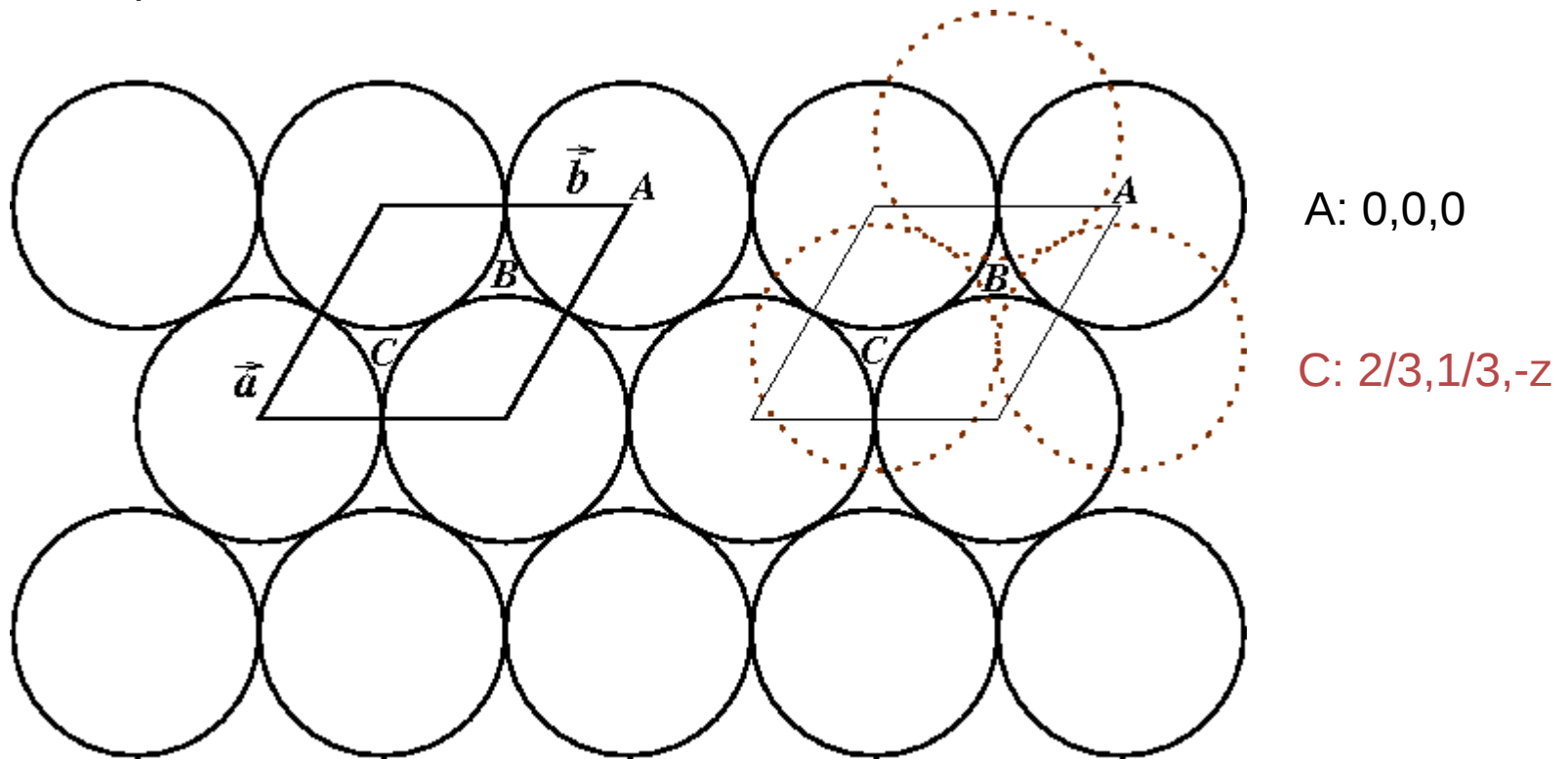
A: 0,0,0

B: $1/3, 2/3, z$

position of atoms in two adjacent layers A B

if repeated periodically ABABAB... hexagonal closest packing

close packed spheres

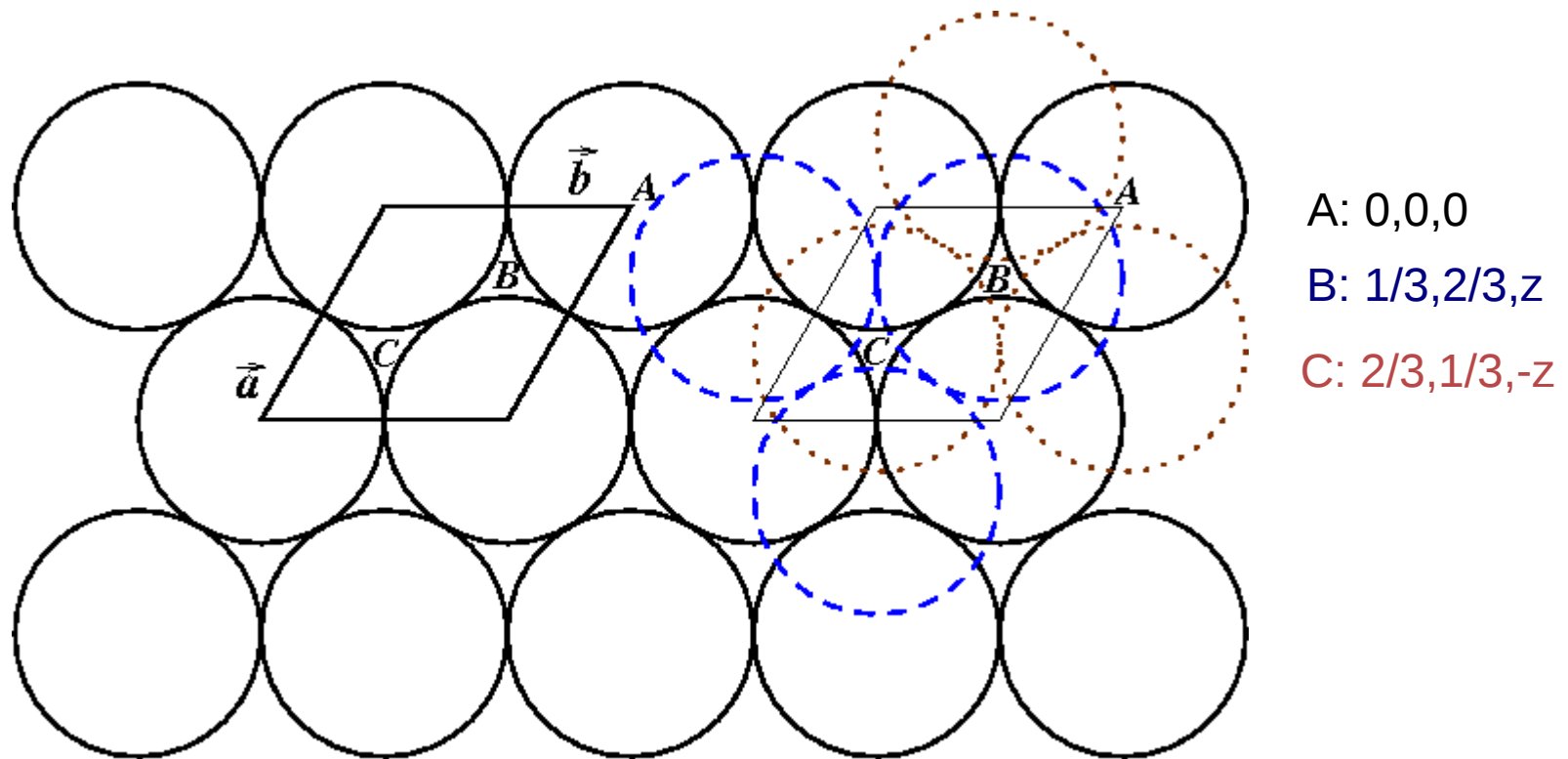


Position of atoms in two adjacent layers A C

if repeated periodically ACACAC... hexagonal close packing

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

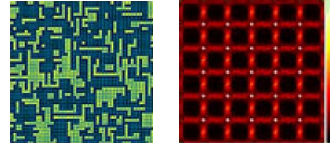
close packed spheres



atom position in three adjacent layers

if repeated periodically ABCABC... closed packed

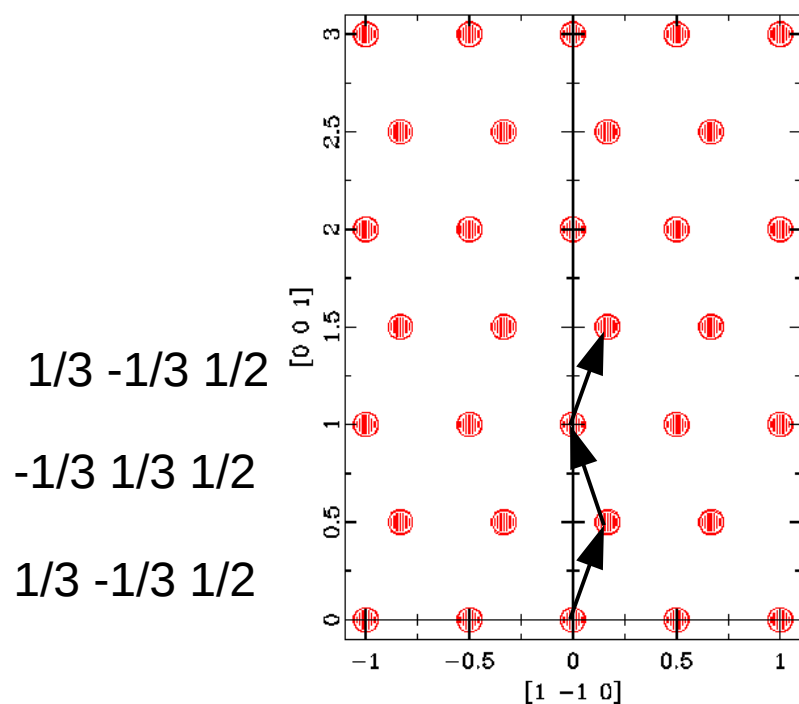
closed packed layer corresponds to **each** of the $\{111\}$ layers !



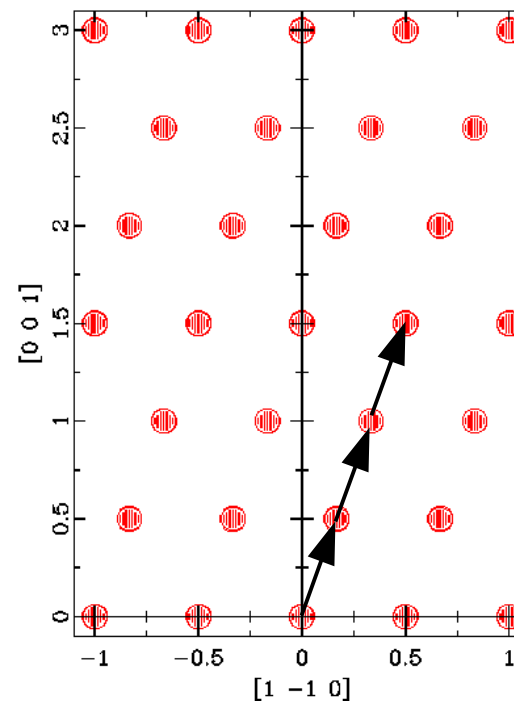
Comparison: HCP <== CCP



layer normal to $[110]$



A A
 B C
 A B
 B A
 A C
 B B
 A A

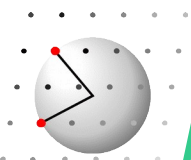


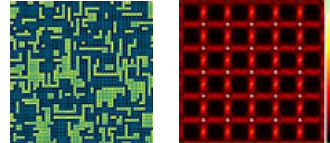
identical sequence of any two adjacent layers
 except for a possible mirror image at $(1-10)$

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

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

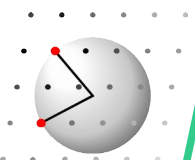
$$F(hkl) = \sum_{atoms} b e^{2\pi i (hx + ky + lz)} \quad z=0 \text{ for all atoms}$$

$$F(hkl) = \sum_{atoms} b e^{2\pi i (hx + ky)} \longrightarrow F(hkl) \text{ independent of } l$$

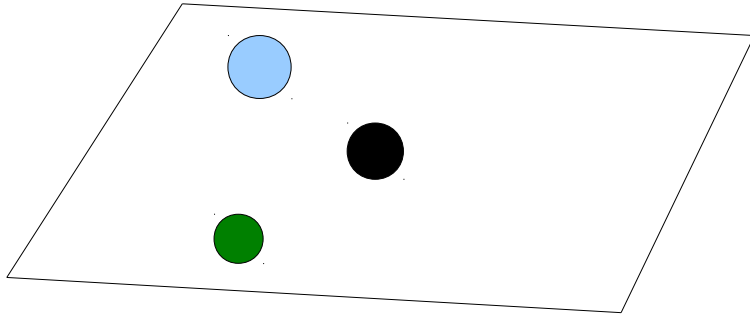
periodic in x and y \longrightarrow $F(hkl) \neq 0$ only for h,k integer

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

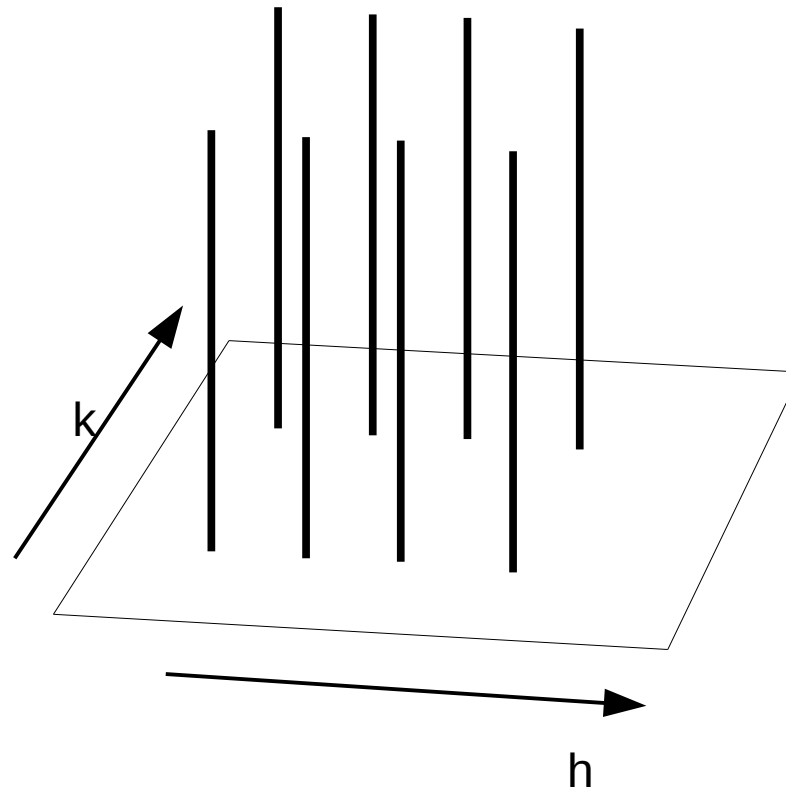
$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{V} \longrightarrow$ rods are normal to the layer



strictly 2-D layer



Fouriertransform





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

crystal = origins of individual layers \otimes atoms with a single layer

\otimes = convolution

Fouriertransform:

$$\mathcal{F}(\text{origins}) * \mathcal{F}(\text{individual layer})$$



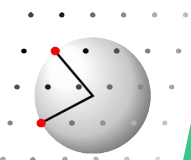
generally a continuous
function in reciprocal space



rods parallel l at h,k integer



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





Stacking faults



example

comparison hexagonal / cubic closed packing

H0L layer in hexagonal metric

Extinction rules

$$00l \quad l=2n$$

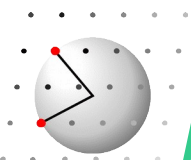
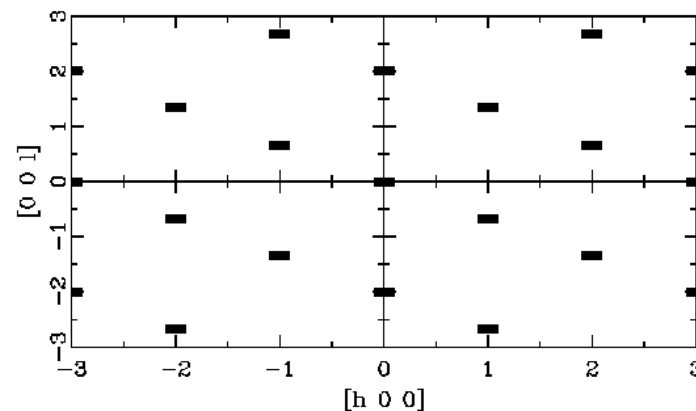
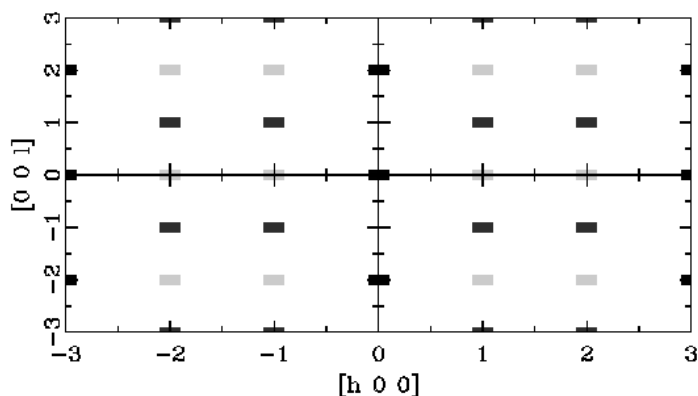
$$hkl \quad l=2n \text{ or}$$

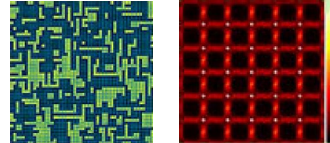
$$h-k = 3n+1 \text{ or}$$

$$h-k = 3n-2$$

$$hkl \quad h,k,l = ggg \text{ or } uuu$$

$$\text{Reflections at} \quad l = n * 2/3$$





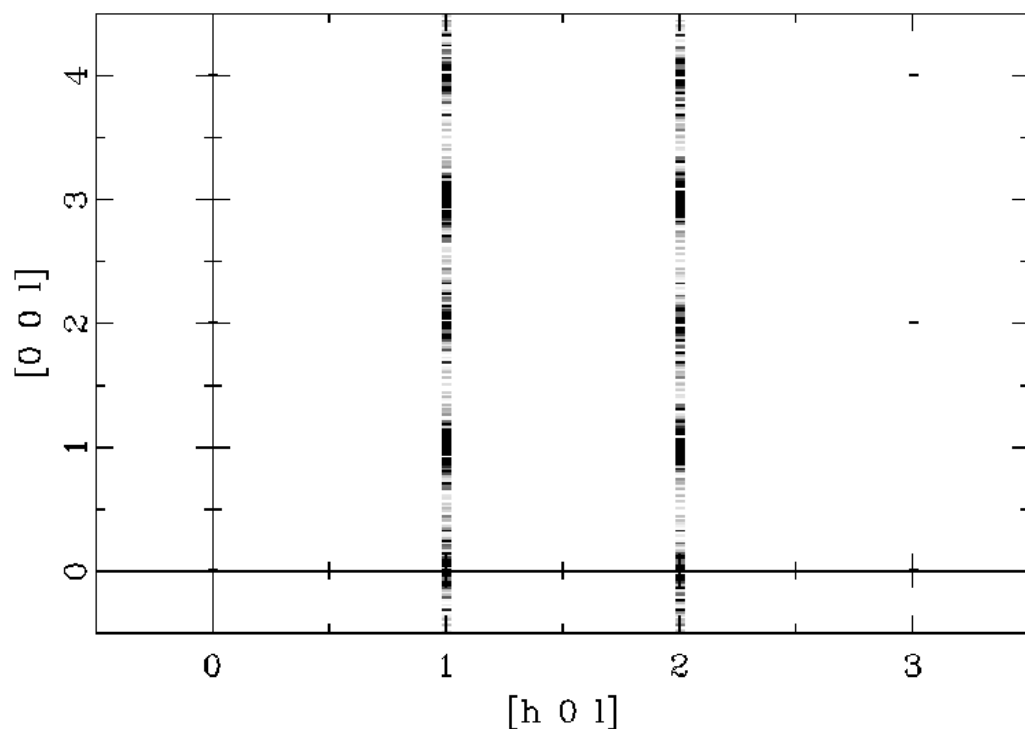
Stacking faults



example

Closed backed spheres, neutron scattering

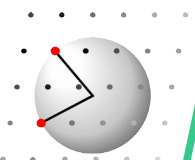
random sequence of layers ABC... with Reichweite 1



H0L layer
metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

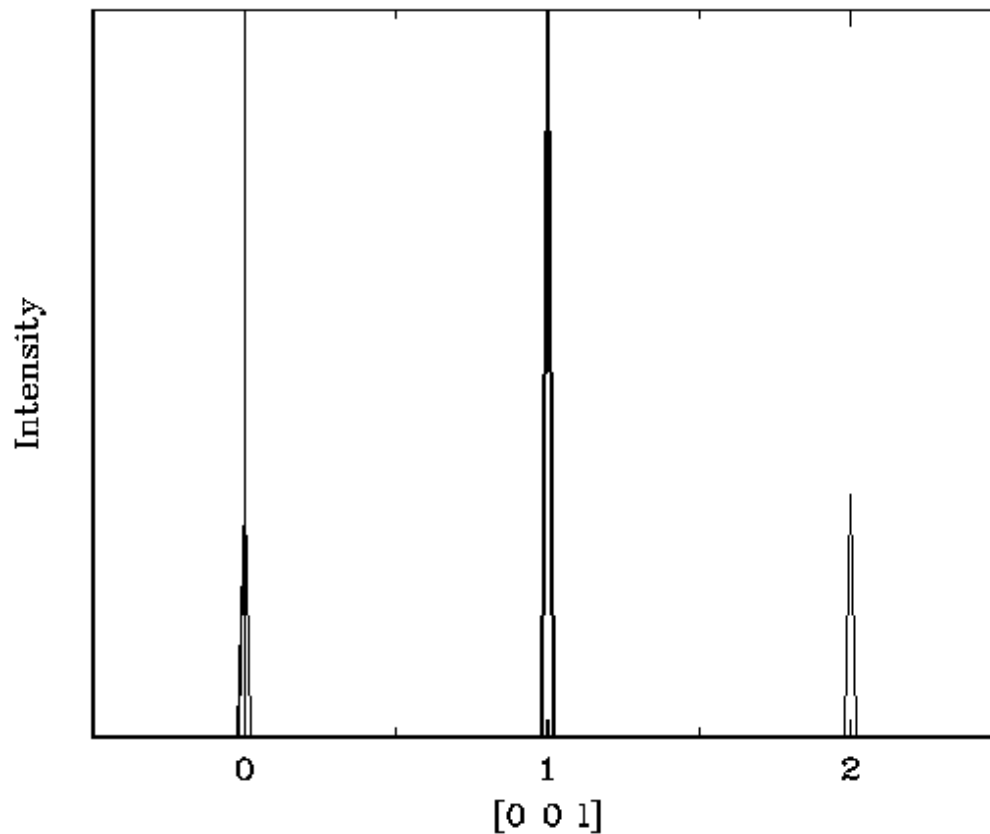
preferred: ABABAB..



example

Closed packed spheres, neutron scattering

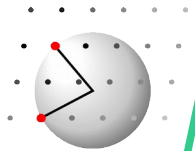
random sequence of layers ABC... with Reichweite 1



H0L layer
metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

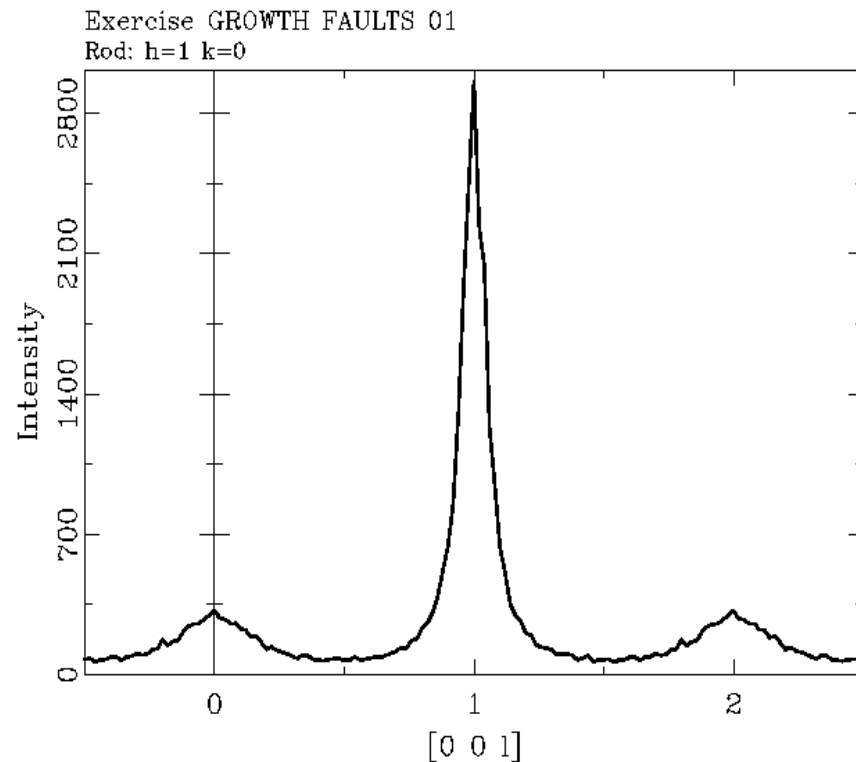
perfect ABAB.. sequence



example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod

Metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

ABAB.. sequence,
25% stacking fault-
probability

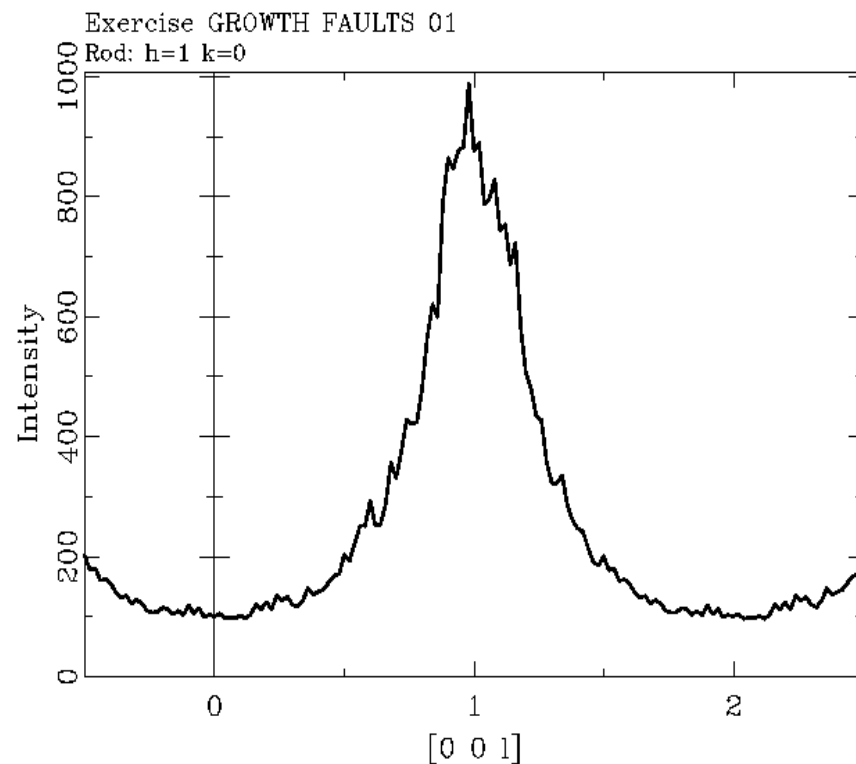
A B 0.75

A C 0.25

example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod

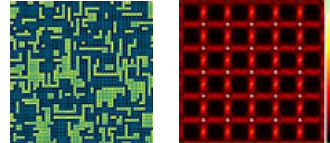
Metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

ABAB.. sequence,
50% stacking fault
probability

A B 0.50

A C 0.50



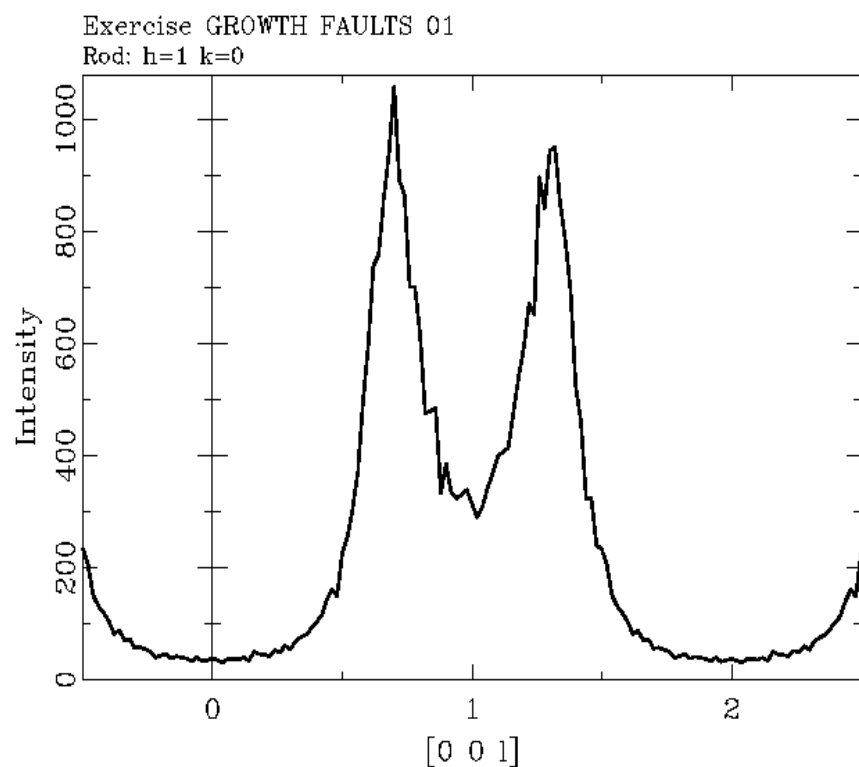
Stacking faults



example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod

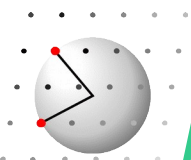
Metric: hexagonal
reciprocal lattice

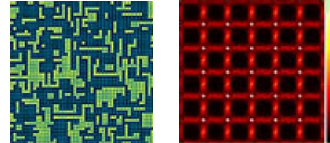
diffuse rods at $h \neq 3n$

ABAB.. sequence,
75% stacking fault
probability

A B 0.25

A C 0.75





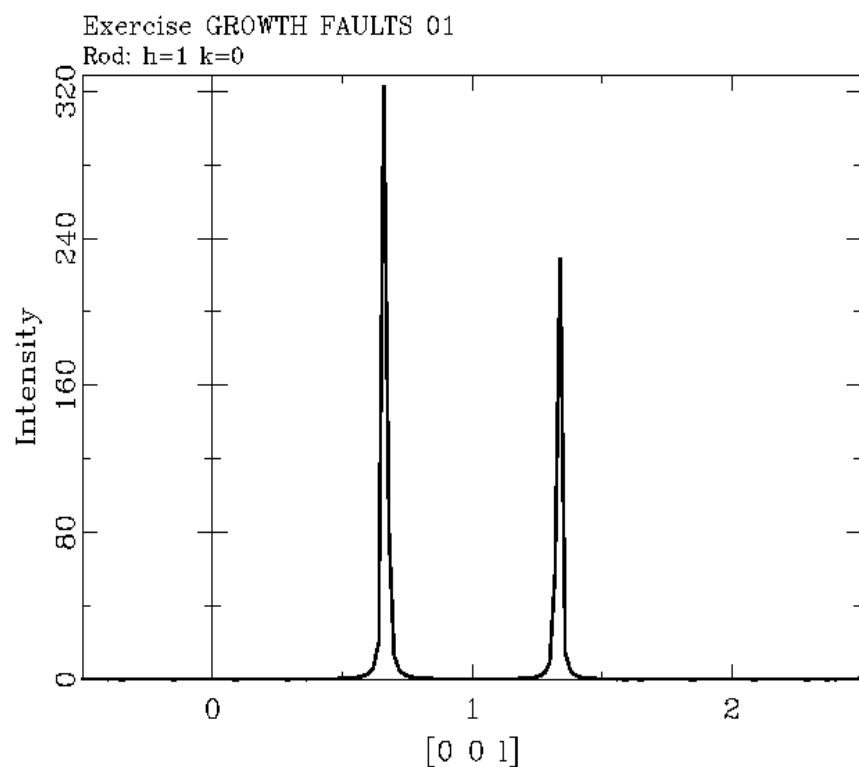
Stacking faults



example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1



10L rod

Metric: hexagonal
reciprocal lattice

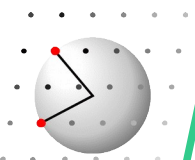
diffuse rods at $h \neq 3n$

ABAB.. sequence,
100% stacking fault
probability

A B 0.00

A C 1.00

Single twinned crystal





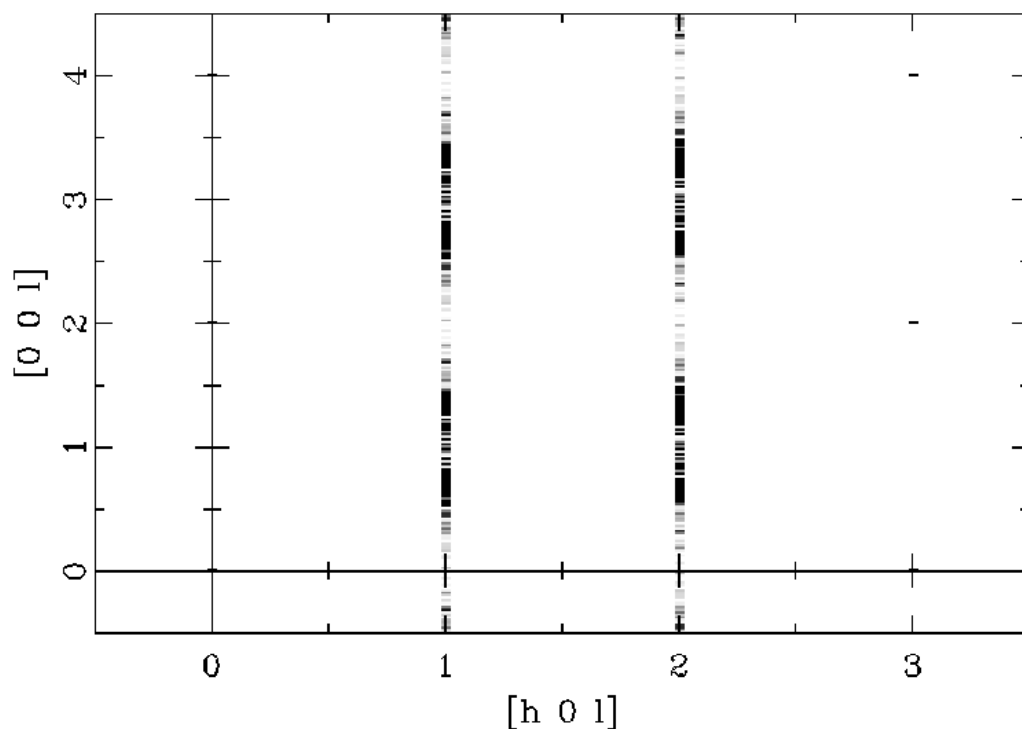
Stacking faults



example

Closed packed spheres, neutron scattering

random sequence of layers ABC... with Reichweite 1

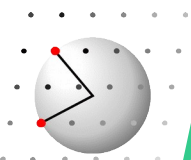


10L rod

Metric: hexagonal
reciprocal lattice

diffuse rods at $h \neq 3n$

preferred ABCABC..





layer types A,B,C, ...

atom positions within each layer type
dependent on layer sequence ?

vectors from layer to layer

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

probabilities for any pair:

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

extend of the interaction

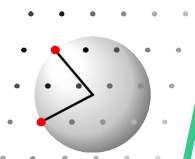
type of layer n is determined by
n-1
n-1, n-2,
n-1, n-2, n-3
...

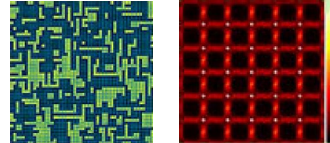
extend of the layers

across the whole crystal

only a partial layer within the crystal
limited by dislocations

all faulted layers parallel to each other ?





Stacking faults: general rules



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

$$\frac{1}{3}\vec{a}$$

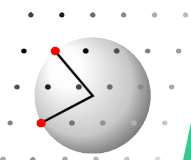
No diffuse scattering at rod 30L

vectors from layer to layer

$$u\vec{a}+v\vec{b}+w\vec{c}$$

No diffuse scattering at rods where

$$uh+vk+wl = 0$$



Run discus_suite

Change to directory:

Lectures\05.Stack\STACK

Use macro: stack.01.mac with one parameter: <fault_probability>

suite> @stack.01.mac 0.0

suite> @stack.01.mac 1.0

**Be creative with the
Parameters between 0 and 1!**

