Reciprocal Lattice
&
Ewald Sphere Construction

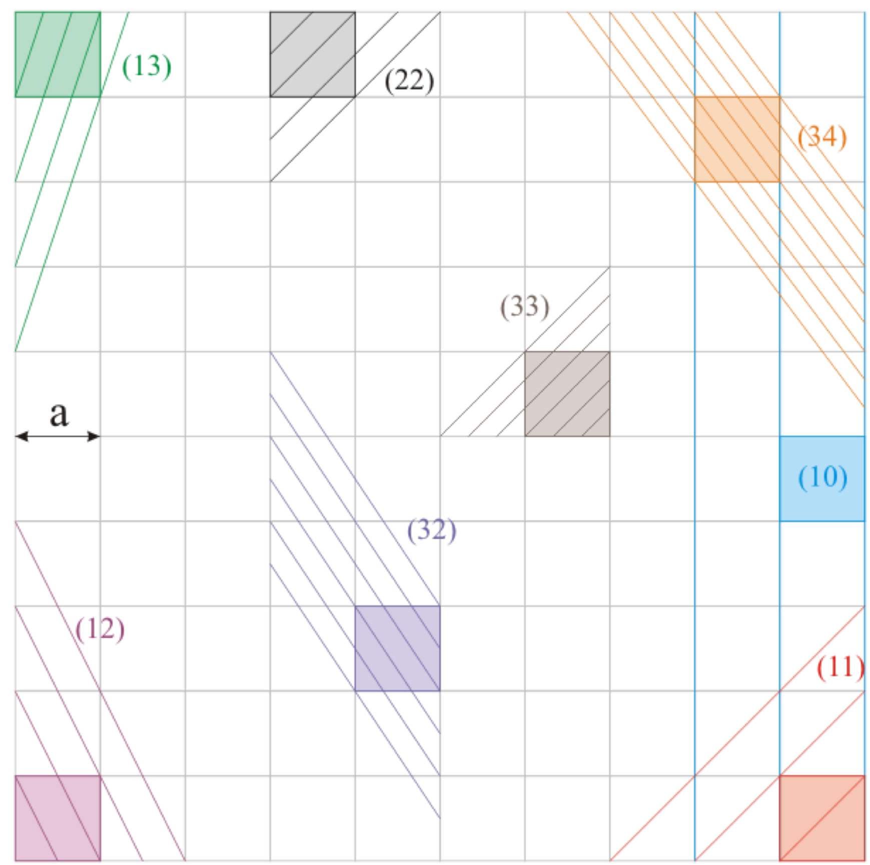
- Reciprocal lattice. Reciprocal Crystal.
- Structure factor calculations.
- Ewald sphere construction.
- Diffraction patterns.

- A crystal resides in real space. The diffraction pattern resides in Reciprocal Space.
- In a diffraction experiment *(e.g. powder diffraction using X-rays, selected area diffraction in a TEM)*, a part of this reciprocal space is usually sampled.
- The diffraction pattern from a crystal (in Fraunhofer diffraction geometry), consists of a periodic array of spots (sharp peaks of intensity).
- From the real lattice the reciprocal lattice can be *geometrically constructed*☺. The properties of the reciprocal lattice are 'inverse' of the real lattice → planes 'far away' in the real crystal are closer to the origin in the reciprocal lattice.
- As a real crystal can be thought of as decoration of a lattice with motif; a reciprocal crystal can be visualized as a Reciprocal Lattice decorated with a motif* of Intensities.
  - **Reciprocal Crystal = Reciprocal Lattice + Intensities as Motif***
- The reciprocal of the 'reciprocal lattice' is nothing but the real lattice!
- *Planes* in real lattice become *points* in reciprocal lattice and vice-versa.

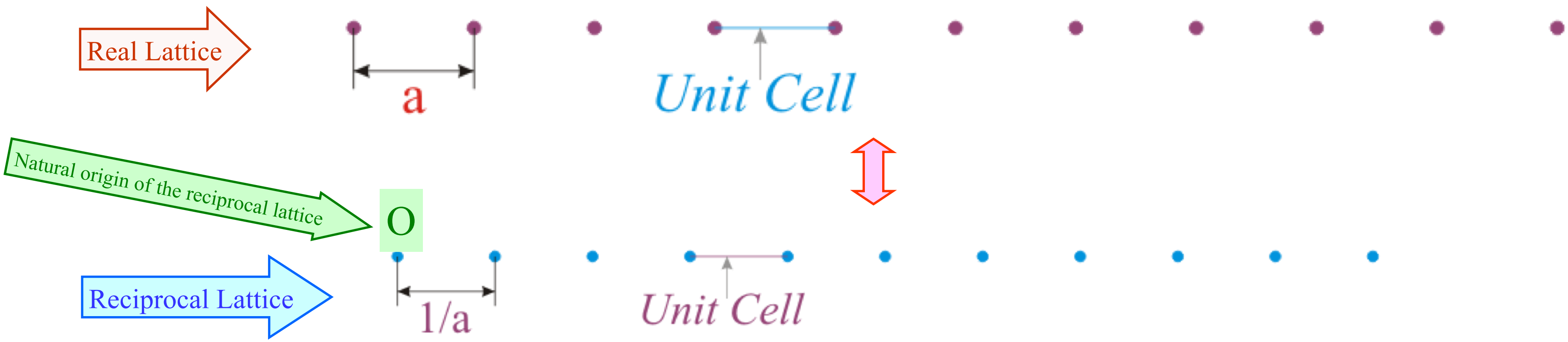
A motivation for constructing reciprocal lattices

- This as you will remember is the Bragg's viewpoint of diffraction. Hence, we would like to have a construction which maps planes in a real crystal as points.
- Apart from the use in 'diffraction studies' we will see that it makes sense to use reciprocal lattice when we are dealing with planes.
- The crystal 'resides' in Real Space, while the diffraction pattern 'lives' in Reciprocal Space.

- As the index of the plane increases
  → the interplanar spacing decreases
  → and 'planes start to crowd' in the real
  ➢ *Hence, it is a 'nice idea' to work in reciprocal space (i.e. work with the reciprocal lattice), especially when dealing with planes.*

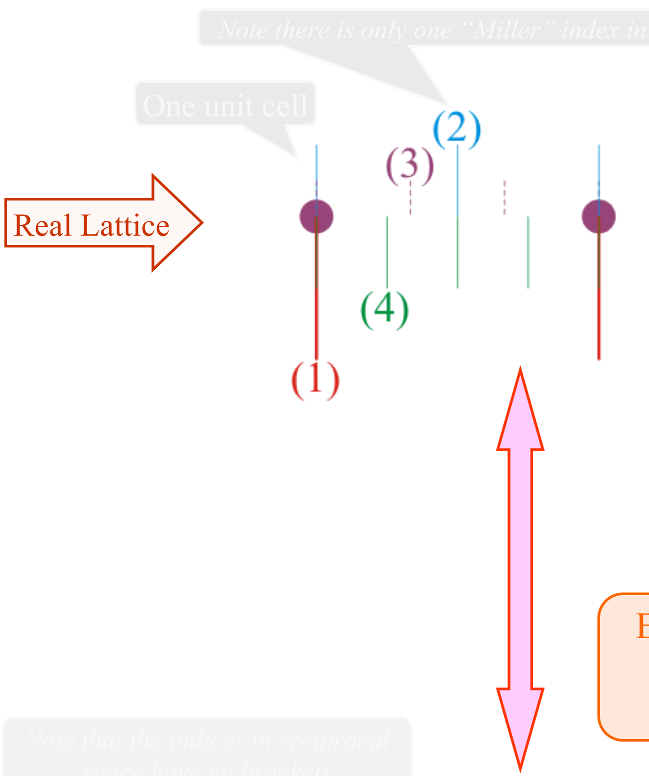


Let us start with a one dimensional lattice and construct the reciprocal lattice

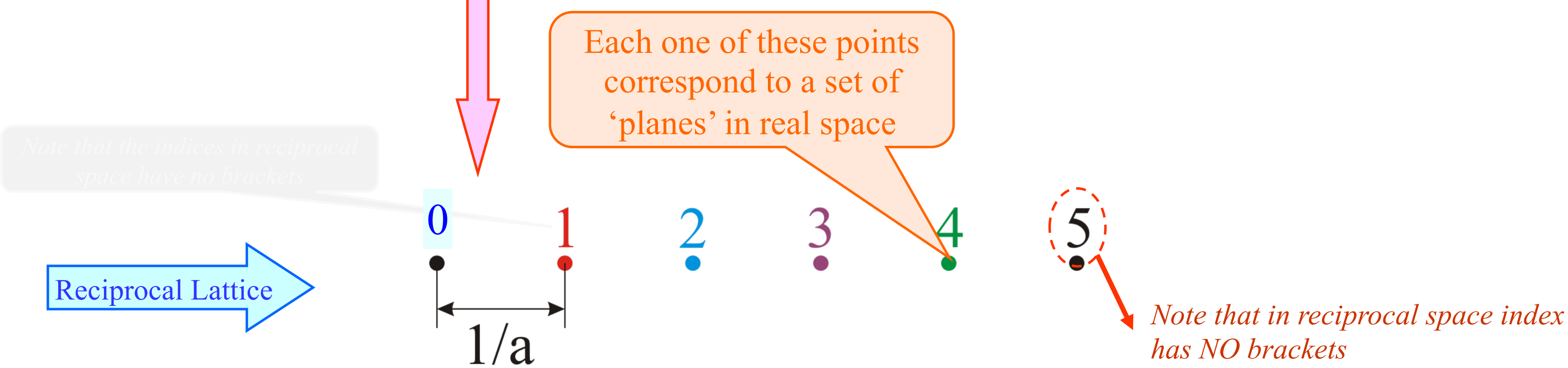


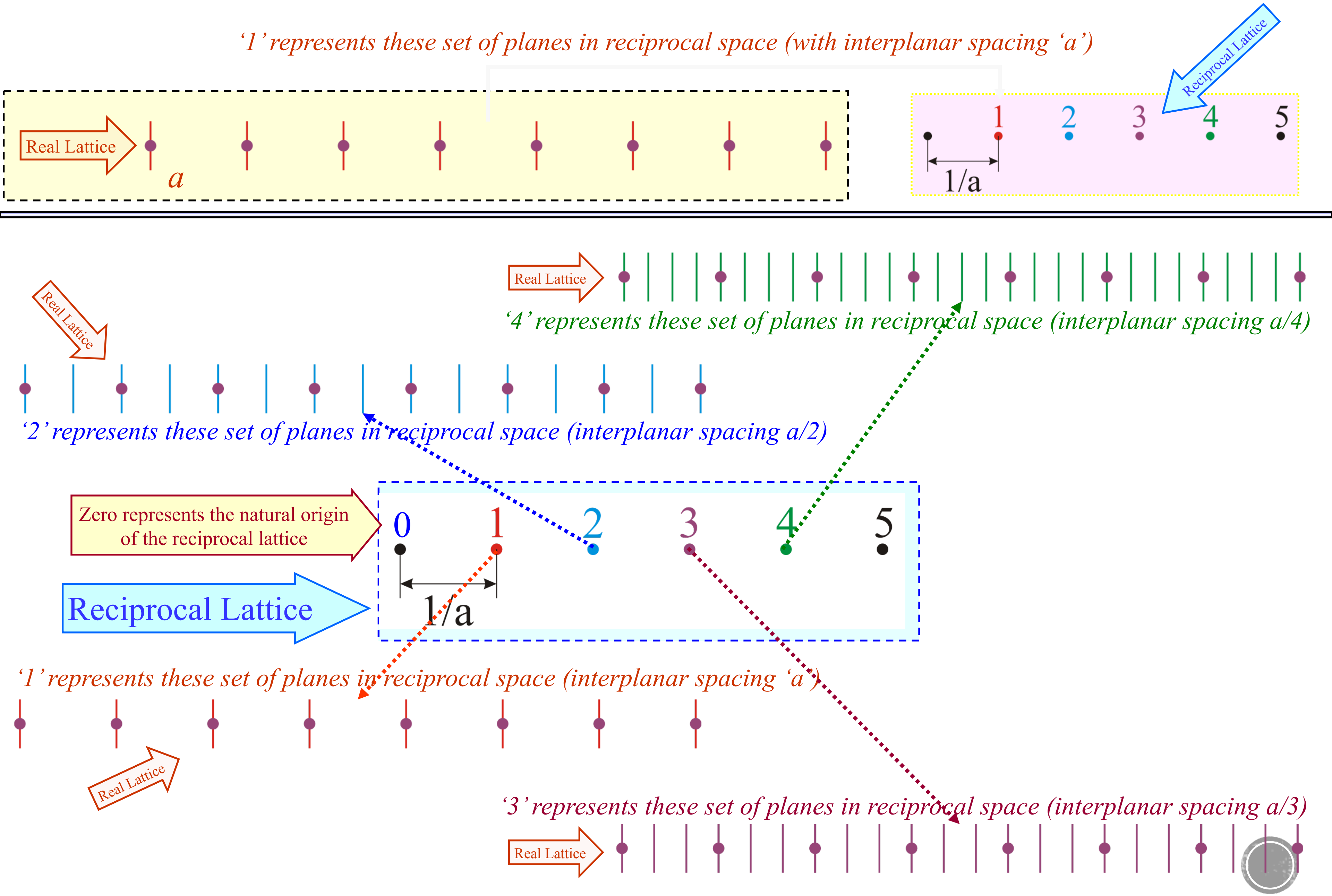
- The periodic array of points with lattice parameter 'a' is transformed to a reciprocal lattice with periodicity of '1/a'.
- The reciprocal lattice point at a distance of 1/a from the origin (O), represents the whole set of points (at a, 2a, 3a, 4a,….) in real space.
- The reciprocal lattice point at '2/a' comes from a set of points with fractional lattice spacing a/2 (i.e. with periodicity of a/2). The lattice with periodicity of 'a' is a subset of this lattice with periodicity of a/2.
- The reciprocal lattice has a natural origin (labelled 'O').

- To construct the reciprocal lattice we need not 'go outside' the unit cell in real space!.
- Just to get a 'feel' for the planes we will be dealing with in the construction of 3D reciprocal lattices, we *'extend'* these points perpendicular to the 1D line and treat them as 'planes'.



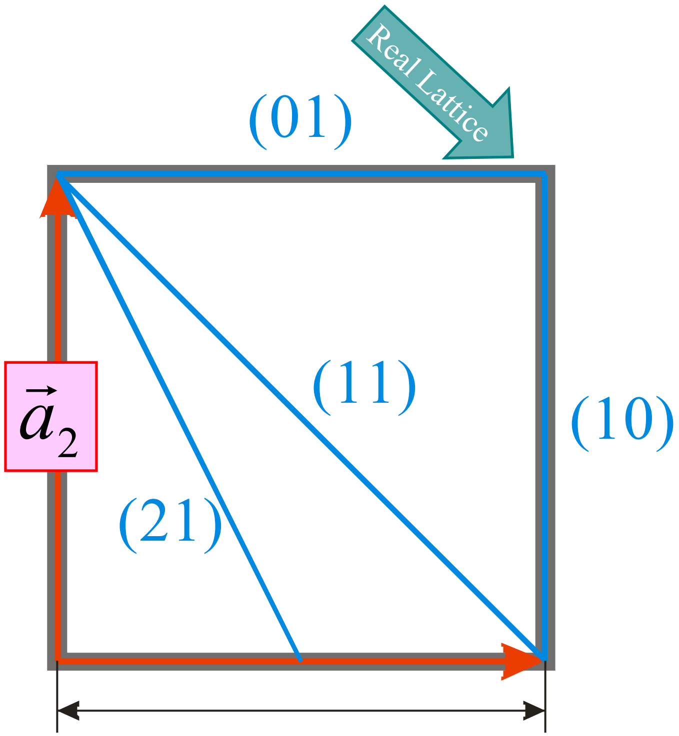
- The plane (2) has intercept at ½, plane (3) has intercept at 1/3 etc.
- As the index of the plane increases the interplanar spacing decreases and the first in the setgets closer to the origin (there is overall crowding).
- *What do these planes with fractional indices mean?*
  - *We have already noted the answer in the topic on Miller indices and XRD.*

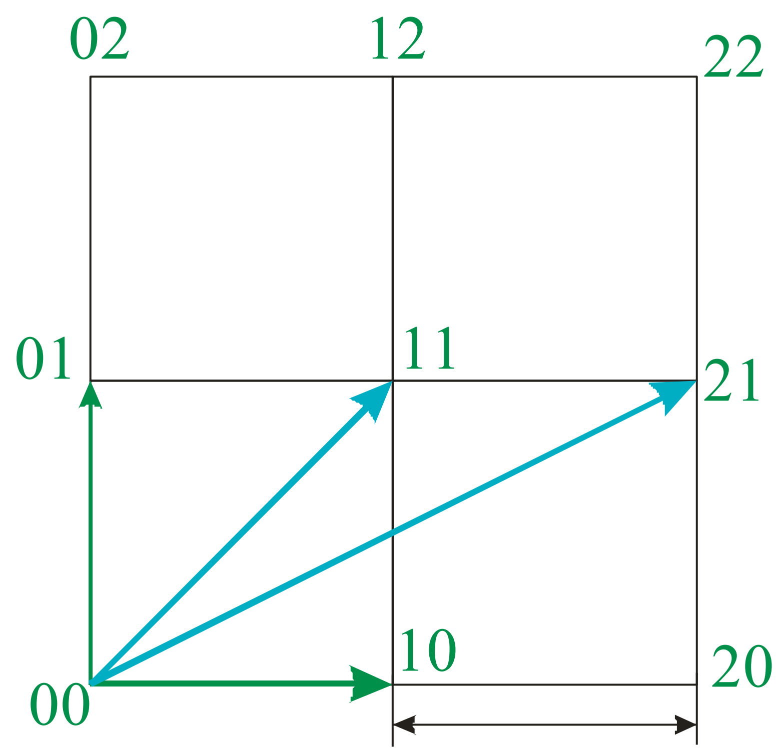




'1' represents these set of planes in reciprocal space (with interplanar spacing 'a')
Real Lattice
a
Reciprocal Lattice
1
2
3
4
5
1/a
Real Lattice
'4' represents these set of planes in reciprocal space (interplanar spacing a/4)
Real Lattice
'2' represents these set of planes in reciprocal space (interplanar spacing a/2)
Zero represents the natural origin of the reciprocal lattice
0
1
2
3
4
5
Reciprocal Lattice
1/a
'1' represents these set of planes in reciprocal space (interplanar spacing 'a')
Real Lattice
'3' represents these set of planes in reciprocal space (interplanar spacing a/3)
Real Lattice

- The square lattice in 2D is defined by two basis vectors (**a**$_1$ & **a**$_2$).
- The planes in 2D$_{\text{real lattice}}$ become points in 2D$_{\text{reciprocal lattice}}$.
- E.g. the (10) plane in real space becomes the *10* point in reciprocal space.
- The basic vectors for the reciprocal lattice are defined by the (10) and (01) planes. I.e. the $\vec{b}_1^*$ is the vector connecting *00* to *10* and the $\vec{b}_2^*$ is the vector connecting *00* to *01*.
- Once we have the basis vectors, we can construct the entire reciprocal lattice.





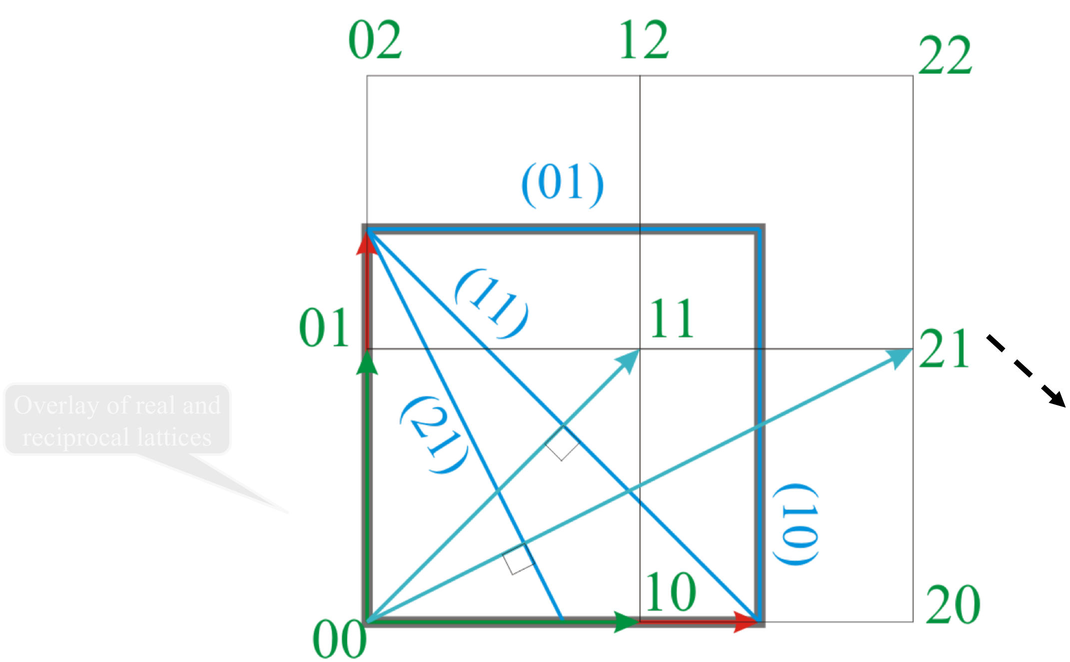
- If we overlay the real and reciprocal lattices then we can see that: *11* vector in reciprocal space is orthogonal to the (11) planes in real space.
- I.e. planes in real space are orthogonal to the corresponding reciprocal lattice vector.

The *11* vector in reciprocal space is : $\vec{g}^{\,*}_{11} = 1 \cdot \vec{b}_1^{\,*} + 1 \cdot \vec{b}_2^{\,*}$

Any general vector in a 2D reciprocal lattice is given by: $\vec{g}^{\,*}_{hk} = h\,\vec{b}_1^{\,*} + k\,\vec{b}_2^{\,*}$

This can be generalized to 3D as: $\vec{g}^{\,*}_{hkl} = h\,\vec{b}_1^{\,*} + k\,\vec{b}_2^{\,*} + l\,\vec{b}_3^{\,*}$

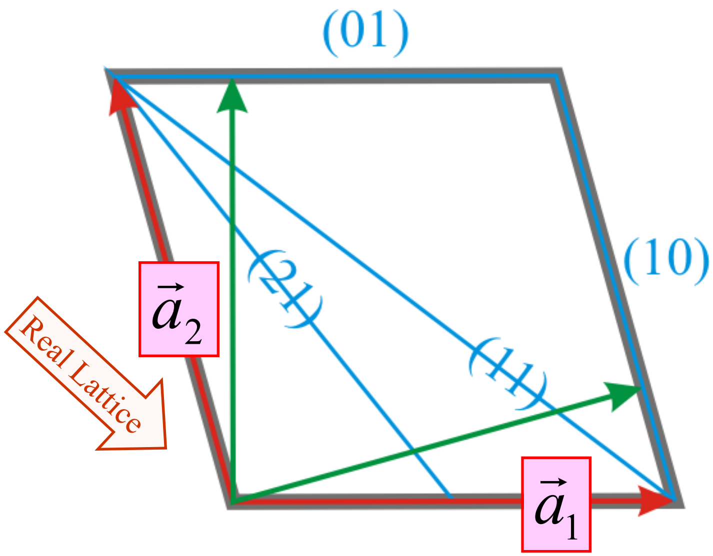
Note that the indices corresponding to the real spaces planes; i.e. h, k & l are retained as subscripts to the vector ***g*** *in the reciprocal space.*

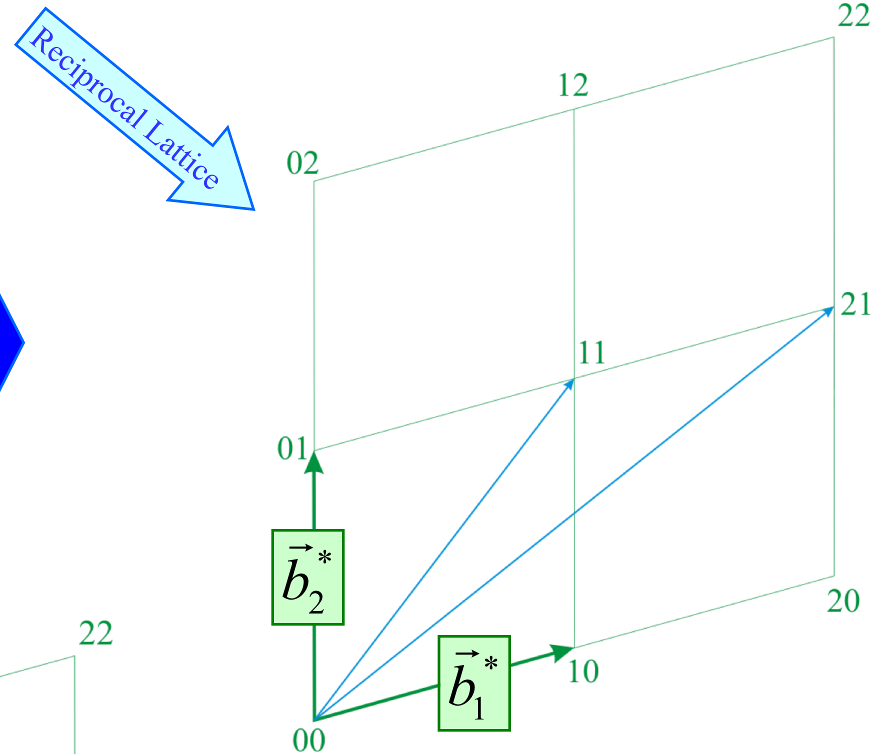


Note that vectors in reciprocal space are perpendicular to planes in real space (as constructed!)

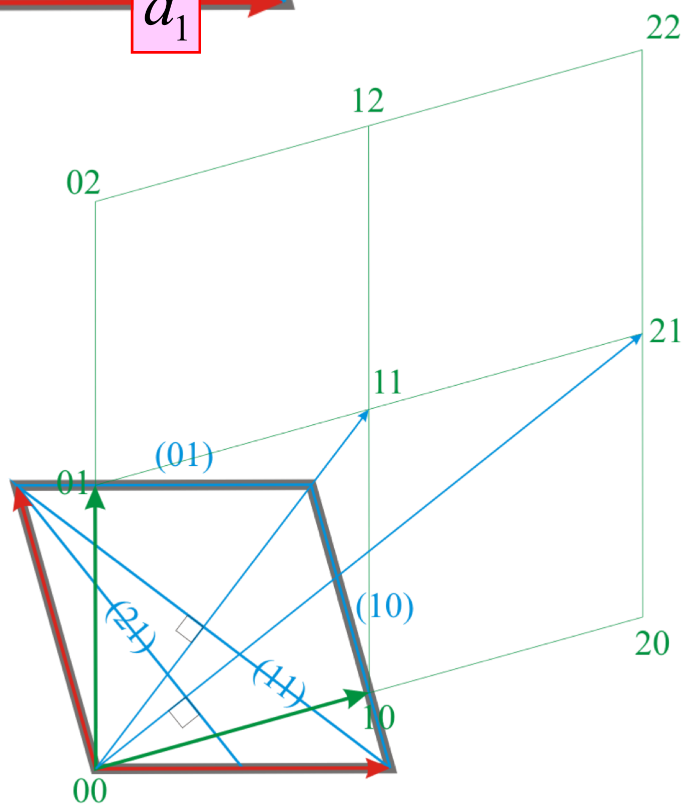
But do not measure distances from the figure!

Example-2 Oblique lattice (parallogram)





The reciprocal lattice



Note that vectors in reciprocal space are perpendicular to planes in real space (as constructed!)

But do not measure distances from the figure!

Reciprocal Lattice (3D)

Properties are reciprocal to the crystal lattice

- To get the reciprocal lattice in 3D, we need 3 basis vectors.
- These are defined using the basis vectors of the crystal as below, where V is the volume of the unit cell.
- The magnitude of the reciprocal lattice basis vector is (1/corresponding interplanar spacing).

BASIS VECTORS

$$\vec{b}_1^* = \frac{1}{V}(\vec{a}_2 \times \vec{a}_3)$$

$$\vec{b}_2^* = \frac{1}{V}(\vec{a}_3 \times \vec{a}_1)$$

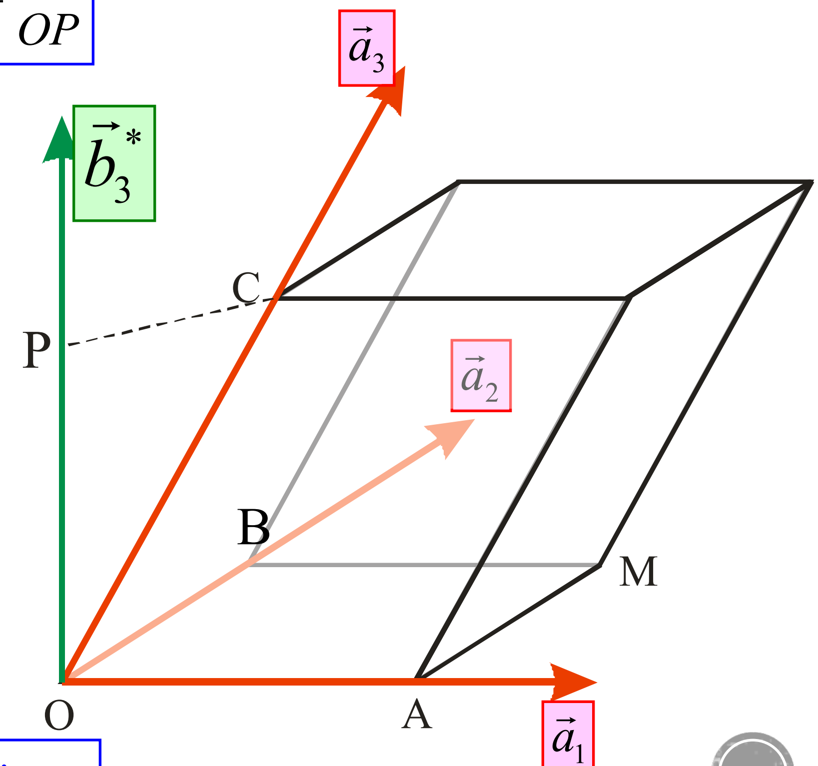
$$\vec{b}_3^* = \frac{1}{V}(\vec{a}_1 \times \vec{a}_2)$$

$\vec{b}_i^*$ is often written as $\vec{a}_i^*$

$$b_3^* = \left|\vec{b}_3^*\right| = \frac{1}{V}\left|(\vec{a}_1 \times \vec{a}_2)\right| = \frac{Area(OAMB)}{Area(OAMB) \cdot Height\ of\ Cell} = \frac{1}{OP}$$

$$b_3^* = \frac{1}{d_{001}}$$

$\vec{b}_3^*$ is $\perp$ to $\vec{a}_1$ *and* $\vec{a}_2$



The reciprocal lattice is created by interplanar spacings

Some properties of the reciprocal lattice and its relation to the real lattice

- A reciprocal lattice vector is $\perp$ to the corresponding real lattice plane

$$\vec{g}^{\,*}_{hkl} = h\,\vec{b}_1^{\,*} + k\,\vec{b}_2^{\,*} + l\,\vec{b}_3^{\,*}$$

- The length of a reciprocal lattice vector is the reciprocal of the spacing of the corresponding real lattice plane

$$g^{*}_{hkl} = \left|\vec{g}^{\,*}_{hkl}\right| = \frac{1}{d_{hkl}}$$

- *Planes in the crystal become lattice points in the reciprocal lattice*
  - *Note that this is an alternate geometrical construction of the real lattice.*
- *Reciprocal lattice point represents the orientation and spacing of a set of planes.*

Notation for basis vectors

Basis vectors in real space → $\vec{a}_1 \quad \vec{a}_2 \quad \vec{a}_3$ *Lattice translation vectors (UC basis vectors)*

Basis vectors in reciprocal space (lattice) → $\vec{b}_1^{\,*} \quad \vec{b}_2^{\,*} \quad \vec{b}_3^{\,*}$ *Reciprocal Lattice translation vectors (UC basis vectors)*

Basis vectors in reciprocal space (crystal) → $\vec{c}_1^{\,*} \quad \vec{c}_2^{\,*} \quad \vec{c}_3^{\,*}$ *Reciprocal Crystal: basis vectors of UC.* *New notation*

"May be" identical to the basis vectors of the reciprocal lattice

General vector in real space → $\vec{r}_{uvw} = ua_1 + va_2 + wa_3$

General vector in reciprocal space → $\vec{g}^{\,*}_{hkl} = h\,\vec{b}_1^{\,*} + k\,\vec{b}_2^{\,*} + l\,\vec{b}_3^{\,*}$

The journey from the real lattice to the diffraction pattern

Crystal = Lattice + Motif

To summarize:

Real Lattice

Decoration of the lattice with motif

Real Crystal

Purely Geometrical Construction

Reciprocal Lattice

Decoration of the reciprocal lattice with Intensities

Structure factor calculation

Reciprocal Crystal

Ewald Sphere construction

*Selection of some spots/intensities from the reciprocal crystal**

Diffraction Pattern**

Diffraction Pattern

Position of the diffraction spots
➢ *RECIPROCAL LATTICE*

Intensity of the diffraction spots
➢ *MOTIF' OF INTENSITIES*

* In fact the Ewald sphere construction selects *regions* of the reciprocal space (which contains the Bragg diffraction pattern from the crystal(s) and diffuse intensities (between the Bragg peaks).

In crystals based on a particular lattice the intensities of particular reflections are modified → *they may even go missing*

** The actual diffraction pattern observed in an experiment depends on the 'detector setup'.

Position of the diffraction spots → Lattice

Intensity of the diffraction spots → Motif

Is determined by

❑**References:** ***MATERIALS SCIENCE & ENGINEERING: A Learner's Guide*, Anandh Subramaniam, http://home.iitk.ac.in/~anandh/E-book.htm.**