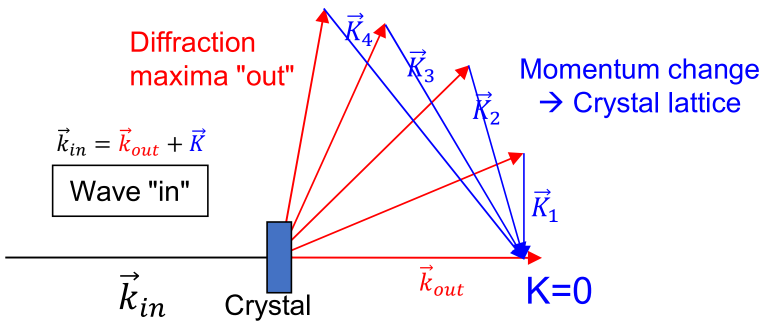
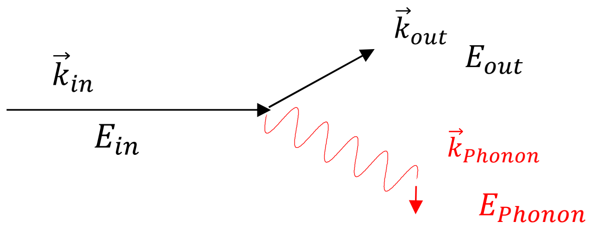
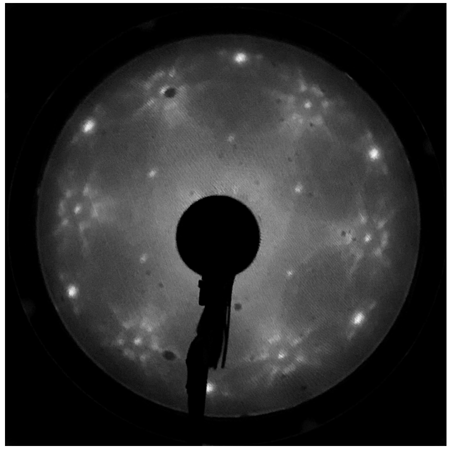
2. Reciprocal lattice

- The **reciprocal lattice** is a Fourier transform of the direct lattice
- Important for:
    1. diffraction experiments
    2. description of the periodicity of the solutions
    3. description of the interactions of waves in solids
    4. description of electronic levels and bands







Low energy electron diffraction (LEED) pattern of ultrathin $Al_2O_3/Ni_3Al(111)$

2. Reciprocal lattice

- **Fourier analysis**: a mathematical technique used to decompose a function or signal into its constituent frequencies.

- Any periodic function can be represented as a sum of simple sinusoidal functions (sines and cosines) with different frequencies, amplitudes, and phases.

- The basic formula for the Fourier series of a function $f(x)$ defined on an interval $[0, L]$ is:

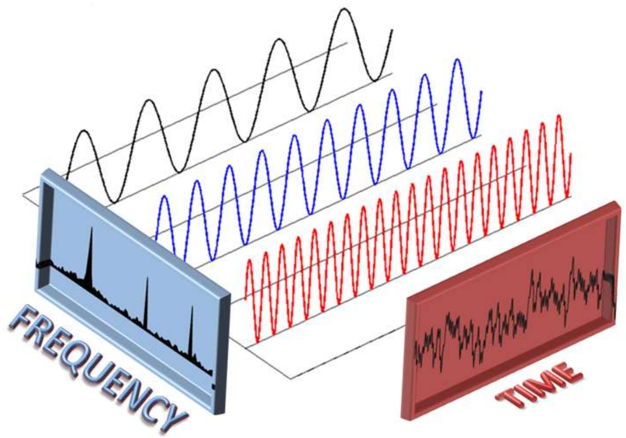
$$f(x) = a_0 + \sum_{n=1}^{+\infty} (a_n cos\left(\frac{2\pi nx}{L}\right) + b_n \sin\left(\frac{2\pi nx}{L}\right)$$

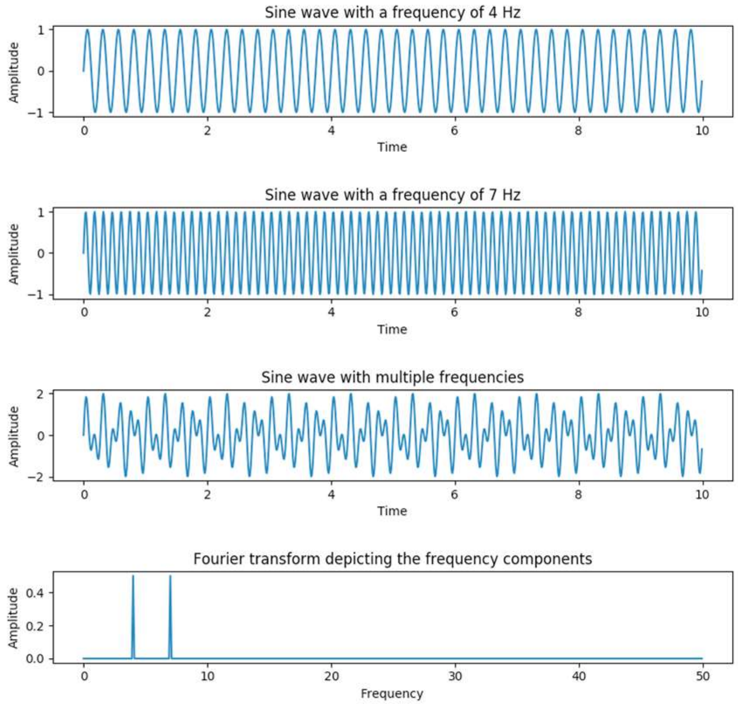
$$= a_0 + \sum_{n=1}^{+\infty} (a_n cos(k_n x) + b_n \sin(k_n x)$$

  Here, a_n and b_n are the Fourier coefficients, which capture the amplitudes of the cosine and sine components.
  $k_n = \frac{2\pi n}{L}$, spatial frequencies.

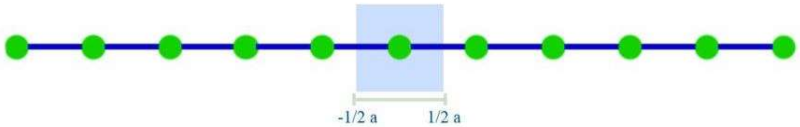
- The basic formula for the Fourier series of a function $f(x)$ defined on an interval $[-\infty, \infty]$ is:

$$f(x) = \int_{-\infty}^{+\infty} \hat{f}(k) e^{2\pi ikx} dk$$





2. Reciprocal lattice



- Consider a simple lattice in one dimension $x_n = na$ with n an integer.
- Two points in k-space (reciprocal space) are equivalent to each other if:
  $k_1 = k_2 + G_m$, where $G_m = \frac{2\pi}{a}m$ with m an integer.
  The points G_m form the **reciprocal lattice**.
- Consider waves of the form:

$$e^{ik\quad_n} = e^{ikna}$$

- Shifting $k \rightarrow k + G_m$ leaves this form unchanged since

$$e^{i(k+G_m)x_n} = e^{i(k+G_m)na} = e^{ikna}e^{i(\frac{2\pi}{a}m)na} = e^{ik\quad_n}$$

$$(e^{i2\pi mn} = 1)$$

$\rightarrow$ So far as the wave is concerned, k is the same as $k + G_m$.

- **Definition**: Given a (direct) lattice of points $\vec{R}$, a point $\vec{G}$ is a point in the reciprocal lattice if and only if:

$$e^{i\vec{G}\cdot\vec{R}} = 1$$

for all points $\vec{R}$ of the direct lattice.

- *The vectors $\vec{G}$ of the reciprocal lattice are all the $\vec{k}$ vectors whose associated plane wave has the periodicity of the direct Bravais lattice.*

2. Reciprocal lattice

Real-space lattice: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Reciprocal lattice: $\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$

- the reciprocal lattice is a lattice in reciprocal space
- the primitive lattice vectors of the reciprocal lattice are defined to have the following property:

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

$$\delta_{ij} = \begin{cases} 1 \ for \ i = j \\ 0 \ for \ i \neq j \end{cases}$$

We can construct vectors $\vec{b}_j$ to have the desired property:

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_2 = 2\pi\frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_3 = 2\pi\frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

It follows that:

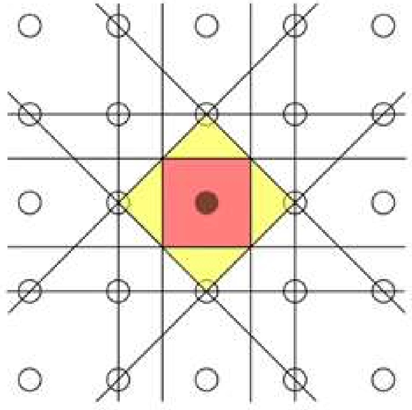
$$\vec{a}_1 \cdot \vec{b}_1 = \vec{a}_1 \cdot 2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi, \qquad \vec{a}_2 \cdot \vec{b}_1 = \vec{a}_2 \cdot 2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0$$

- The points of the reciprocal lattice we must show that $\vec{R} \cdot \vec{K} = 2\pi\delta_{ij}$ is satisfied for all points of the real-space lattice:

$$e^{i\vec{K}\cdot\vec{R}} = e^{i(m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3)\cdot(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)} = e^{2\pi n i}$$

where m_1, m_2, m_3 must be then integer.

2. Reciprocal lattice: Brillouin zone



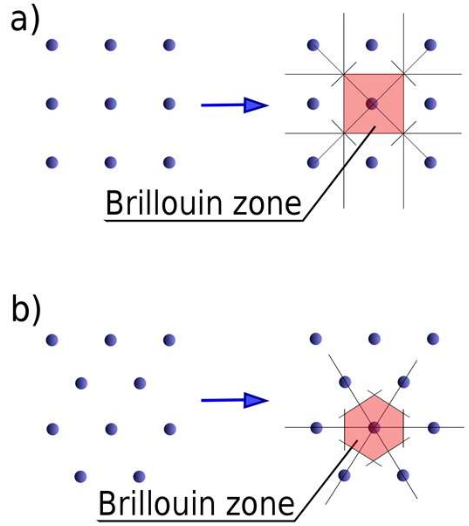
- **Brillouin zone**: the Wigner-Seitz cell of the reciprocal lattice.
- The primitive unit cell of direct lattice has volume:

$$V_{dire} \quad = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3),$$

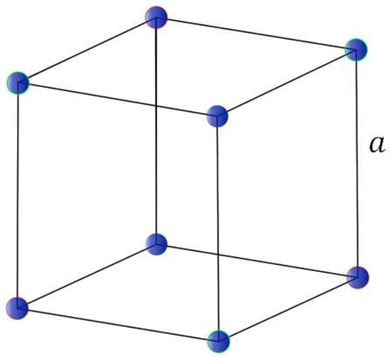
- The reciprocal lattice has volume:

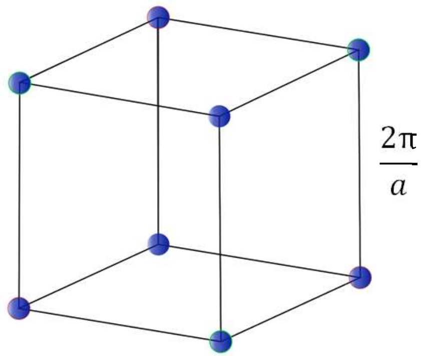
$$V_{reciprocal} = \vec{b}_1 \cdot \left(\vec{b}_2 \times \vec{b}_3\right)$$

- Construction of the first Brillouin zone for a lattice in two dimensions:
  1. First draw a number of vectors from one lattice site to nearby points in the reciprocal lattice.
  2. Next construct lines perpendicular to these vectors at their midpoints.
  3. The smallest enclosed area is the first Brillouin zone.



2. Reciprocal lattice: simple cubic





- The primitive translation vectors of a simple cubic lattice may be taken as the set: $\vec{a}_1 = a_1\vec{e}_x, \vec{a}_2 = a_2\vec{e}_y, \vec{a}_3 = a_3\vec{e}_z$
- The volume of the cell is: $V = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = a^3$
- The primitive translation vectors of the reciprocal lattice are: $\vec{b}_1 = \left(\frac{2\pi}{a}\right)\vec{e}_x, \vec{b}_2 = \left(\frac{2\pi}{a}\right)\vec{e}_y, \vec{b}_3 = \left(\frac{2\pi}{a}\right)\vec{e}_z$

→ The reciprocal lattice is a simple cubic lattice of lattice constant $\frac{2\pi}{a}$.

- The boundaries of the first Brillouin zones are the planes normal to the six reciprocal lattice vectors at their midpoints.
- The volume of the BZ is $V = \left(\frac{2\pi}{a}\right)^3$

2. Reciprocal lattice: bcc

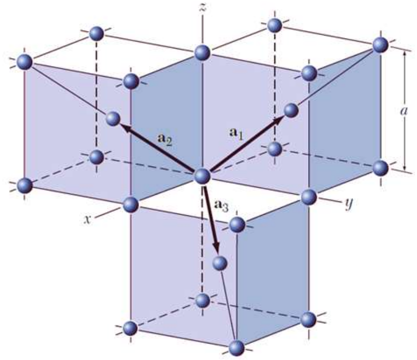
- The primitive vectors of a bcc lattice are: $\vec{a}_1 = \frac{1}{2}a(-\vec{e}_x + \vec{e}_y + \vec{e}_z), \vec{a}_2 = \frac{1}{2}a(\vec{e}_x - \vec{e}_y + \vec{e}_z), \vec{a}_3 = \frac{1}{2}a(\vec{e}_x + \vec{e}_y - \vec{e}_z)$

- The volume of the cell is: $V = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \frac{1}{2}a^3$

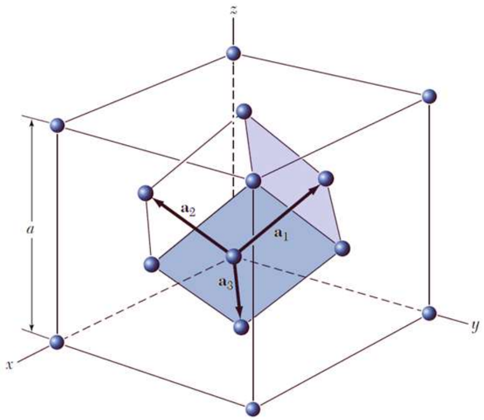
- The primitive vectors of the reciprocal lattice are: $\vec{b}_1 = \left(\frac{2\pi}{a}\right)(\vec{e}_y + \vec{e}_z), \vec{b}_2 = \left(\frac{2\pi}{a}\right)(\vec{e}_x + \vec{e}_z), \vec{b}_3 = \left(\frac{2\pi}{a}\right)(\vec{e}_x + \vec{e}_y)$

→ A fcc lattice is the reciprocal lattice of the bcc lattice.

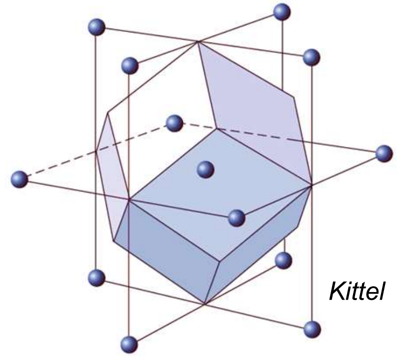
- The volume of the BZ is $V = 2\left(\frac{2\pi}{a}\right)^3$



Primitive basis vectors of the bcc lattice



Primitive basis vectors of the fcc lattice



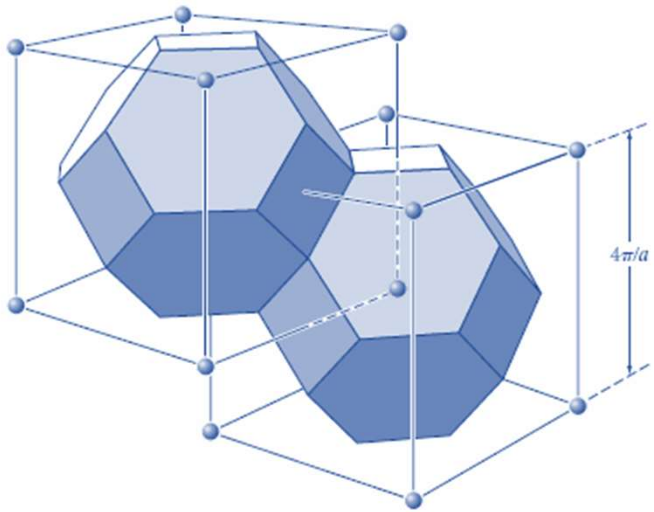
First Brillouin zone of the bcc lattice (regular rhombic dodecahedron)

2. Reciprocal lattice: fcc

- The primitive vectors of a fcc lattice are: $\vec{a}_1 = \frac{1}{2}a(\vec{e}_y + \vec{e}_z), \vec{a}_2 = \frac{1}{2}a(\vec{e}_x + \vec{e}_z), \vec{a}_3 = \frac{1}{2}a(\vec{e}_x + \vec{e}_y)$
- The volume of the cell is: $V = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \frac{1}{4}a^3$
- The primitive vectors of the reciprocal lattice are: $\vec{b}_1 = \left(\frac{2\pi}{a}\right)(-\vec{e}_x + \vec{e}_y + \vec{e}_z), \vec{b}_2 = \left(\frac{2\pi}{a}\right)(\vec{e}_x - \vec{e}_y + \vec{e}_z), \vec{b}_3 = \left(\frac{2\pi}{a}\right)(\vec{e}_x + \vec{e}_y - \vec{e}_z)$

→ A bcc lattice is the reciprocal lattice of the fcc lattice.

- The volume of the BZ is $V = \left(\frac{4\pi}{a}\right)^3$



Brillouin zones of
the fcc lattice.
The cells are in reciprocal space,
and the reciprocal lattice is body
centered.

2. Miller indices

- The conventional notation for describing lattice planes is known as the **Miller indices**:

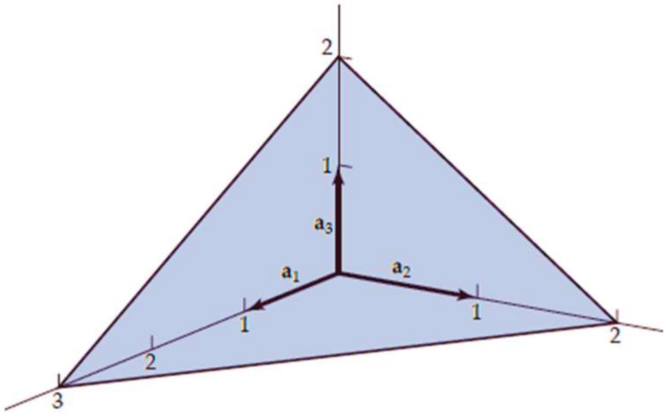
(hkl)

with integers *h, k* and *l*, to mean a family of lattice planes corresponding to reciprocal lattice vector:

$$G_{(hkl)} = hb_1 + kb_2 + lb_3,$$

where b_i are the standard primitive lattice vectors of the reciprocal lattice.

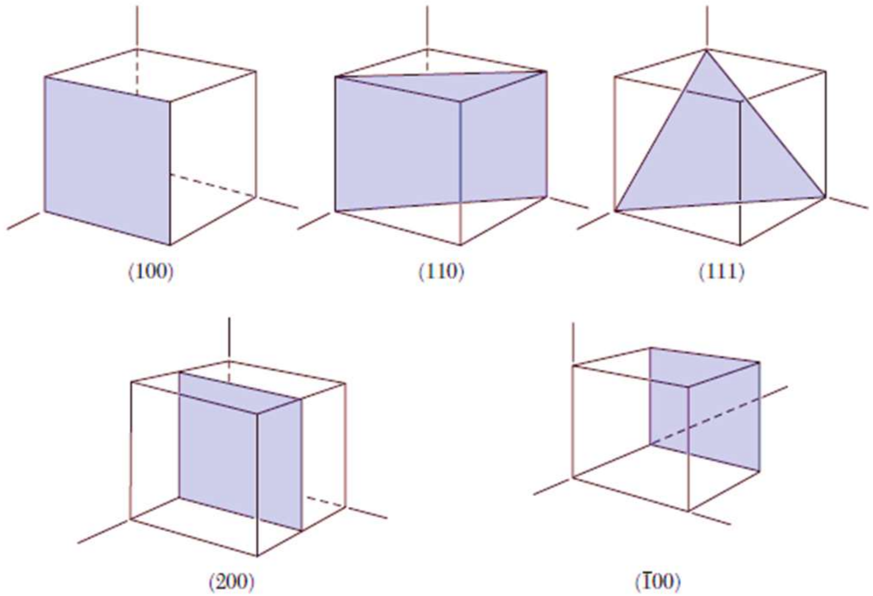
- The orientation of a crystal plane is determined by three points in the plane, provided they are not collinear.
- Specify the orientation of a plane in real space by the Miller indices by the following rules:
    1. Find the intercepts on the axes in terms of the lattice constants a_1, a_2, a_3.
    2. Take the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest three integers.
    3. The results, enclosed in parentheses (*hkl*), are called the Miller indexes of the plane.



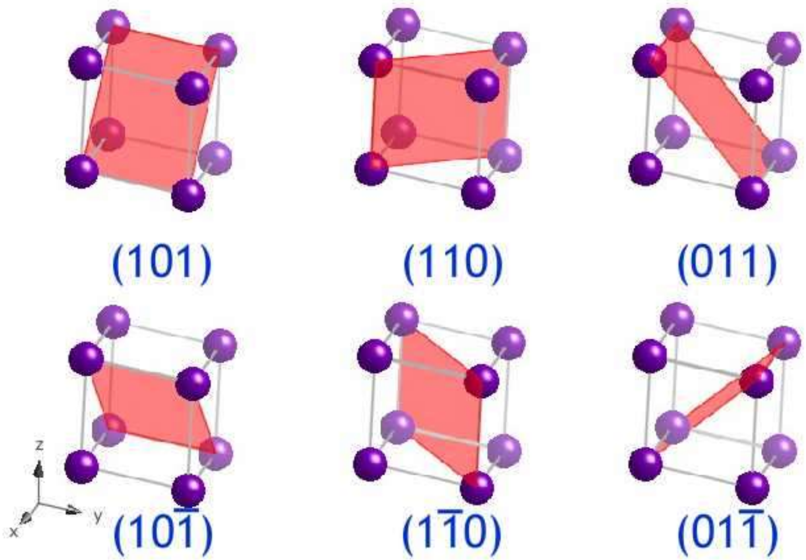
Example:
This plane intercepts the x,y,z axes at $3a_1$, $2a_2$, $2a_3$. The reciprocals of these numbers are 1/3,1/,1/2. The smallest three integers having the same ratio are 2, 3, 3, and thus the indexes of the plane are (233)

2. Miller indices

Example: simple cubic lattice



Family of lattice planes
e.g., {110}

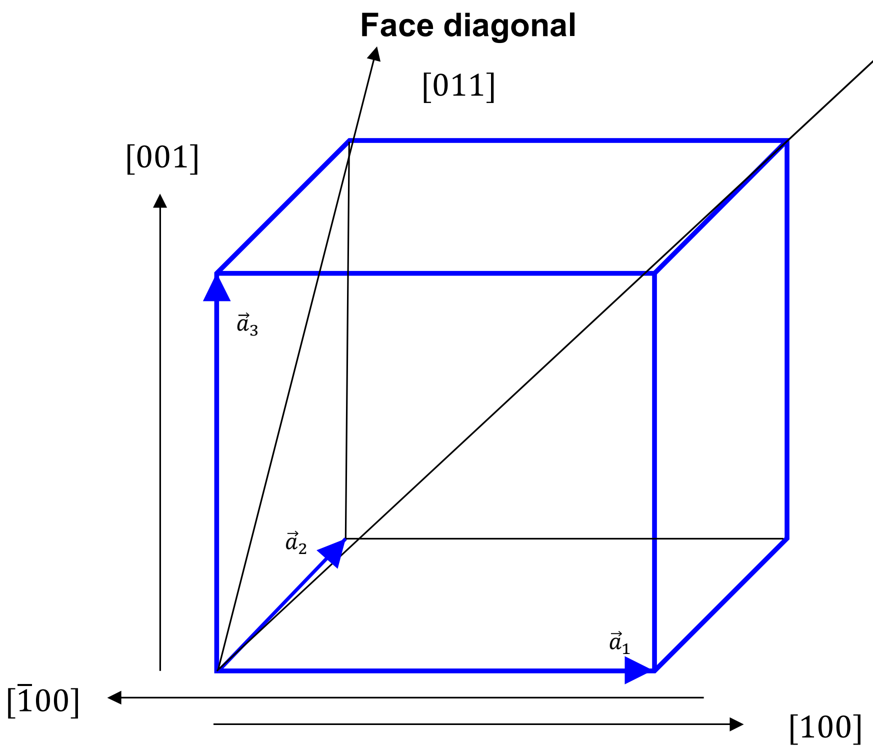


<u>Note</u>: (*hkl*) should be the shortest reciprocal lattice vector in that direction, meaning that the integers *h, k* and *l* should have no common divisor.

One may also write (*hkl*) where h, k and l do have a common divisor, but then one is talking about a reciprocal lattice vector (see next chapter on X-ray diffraction).

2. Crystallographic directions

Example: simple cubic lattice



Family of symmetry-equivalent directions:

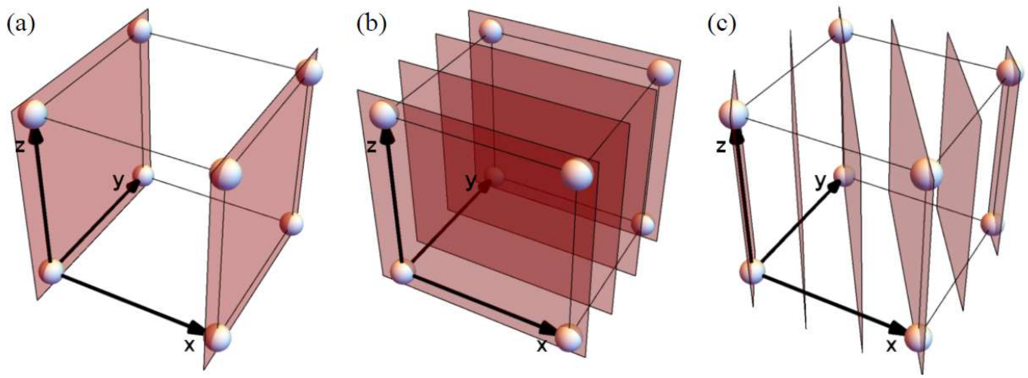
$$< 100 > = [100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]$$

$$(hkl) \perp [hkl]$$

The crystal plane defined as (hkl) is orthogonal to the $[hkl]$ direction.
Correspondence between crystal planes and crystal directions.

2. Families of Lattice Planes

- **Lattice plane**: a plane containing at least three noncolinear (and therefore an infinite number of) points of a lattice
- **Family of lattice planes**: an infinite set of equally separated lattice planes which taken together contain all points of the lattice



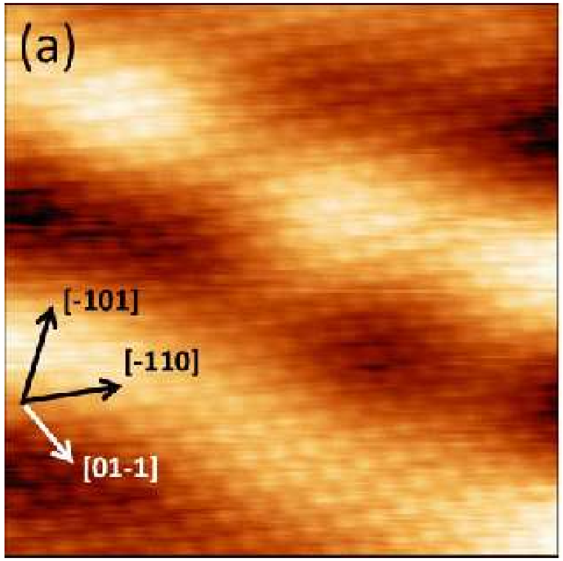
- **The families of lattice planes are in one-to-one with the possible directions of reciprocal lattice vectors, to which they are normal.** The spacing between these lattice planes is:

$$d = 2\pi/|G_{min}| = a/\sqrt{h^2 + k^2 + l^2}$$

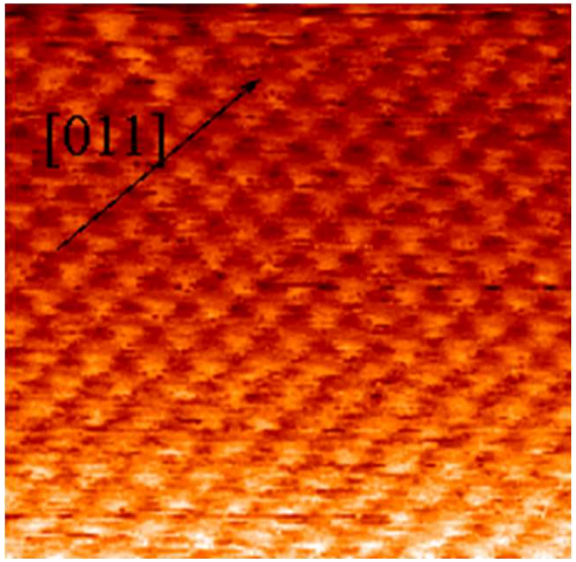
where G_{min} is the minimum length reciprocal lattice vector in this normal direction, and hkl the Miller indices.

2. Miller indices

Scanning Tunneling Microscopy images of atomically flat metal surfaces



Au(111)



Cu(100)

2. AR-based visualization of Miller planes

Visualizing crystal structures and lattice through augmented reality:

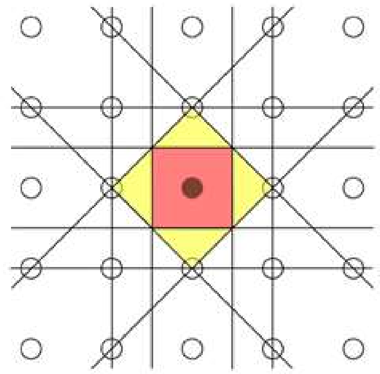
1. Scan the QR code
2. Look at the square with the camera
3. Select the structure
4. Select unit cell (primitive, fcc, bcc)
5. Define Miller indices

2. Reciprocal lattice: summary

Reciprocal lattice: $\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$

Reciprocal lattice vectors:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$



- **Brillouin zone**: the Wigner-Seitz cell of the reciprocal lattice.

- The reciprocal lattice has volume:

$$V_{reciprocal} = \vec{b}_1 \cdot \left(\vec{b}_2 \times \vec{b}_3\right)$$

- **Miller indices**: *(hkl)*

Refer to a family of lattice planes corresponding to reciprocal lattice vector:

$$G_{(hkl)} = hb_1 + kb_2 + lb_3,$$

where b_i are the standard primitive lattice vectors of the reciprocal lattice.