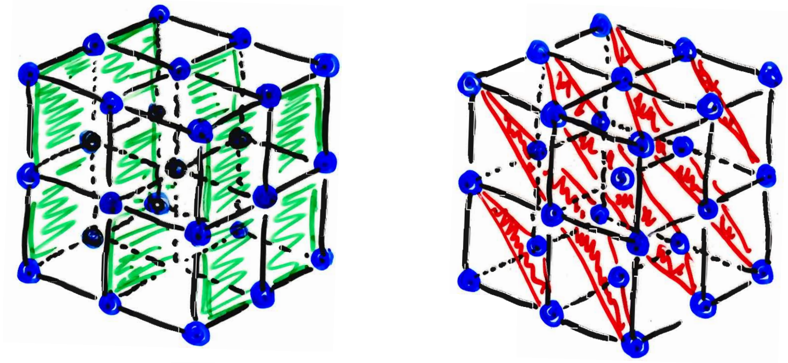
Lattice Planes and Miller Indices

I. $\vec{K}$, reciprocal vectors $\Longleftrightarrow$ Planes of lattice points



1. Take a particular BL
2. Choose 3 noncollinear BL pts

$\Rightarrow$ Get a lattice plane: contains ∞ number of BL pts (translational symmetry)

is a **2D** BL itself (spanned by **2** vectors)

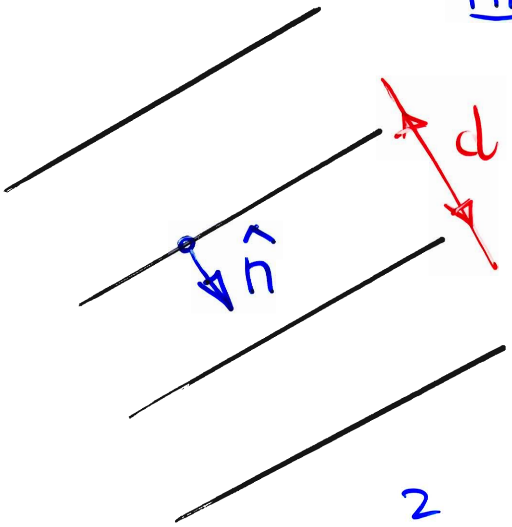
3D BL = family of lattice planes

a set of parallel, equally spaced lattice planes

How to classify different families?

By reciprocal lattice vectors $\vec{K}$!

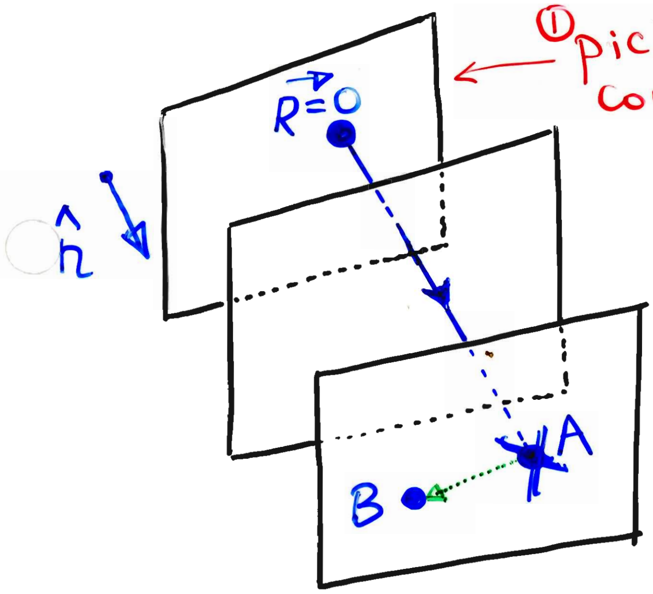
Theorem: $\vec{K}' = \frac{2\pi}{d}\hat{n}$



$\boxed{1}$ $\vec{K}' \in RL$

$\boxed{2}$ $\vec{K}'$ is the shortest RL vector $\parallel \hat{n}$

$\boxed{1}$ $\vec{K}' \overset{?}{\in} RL \iff e^{i\vec{K}'\cdot\vec{R}} \overset{?}{=} 1 \quad \forall \vec{R} \in BL$



① pick out the plane that contains the $\vec{R}=0$ lattice point.

Note $\left. e^{i\vec{K}'\cdot\vec{R}} \right|_{\vec{R}=0} = 1$

② Consider point A

$\vec{R}_A = \hat{n}\, d N$, $\forall$ N-integer

$e^{i\vec{K}'\cdot\vec{R}_A} = e^{i\frac{2\pi}{d}\hat{n}\cdot\hat{n} d N} = 1$

③ Consider $\forall$ point B

$\vec{R}_B = \vec{R}_A + m_1\vec{a}_1 + m_2\vec{a}_2$ parametrize position of B within the plane

m_1, m_2 integers

$\vec{a}_1\cdot\hat{n} = \vec{a}_2\cdot\hat{n} = 0$

$e^{i\vec{K}'\cdot\vec{R}_B} = e^{i\vec{K}'\cdot(\vec{R}_A + m_1\vec{a}_1 + m_2\vec{a}_2)} = e^{i\vec{K}'\cdot\vec{R}_A} = 1$ $\boxed{1}$ ✓

$\boxed{2}$ $|\vec{K}''| < |\vec{K}'|$ would give $\lambda'' > \lambda' = \frac{2\pi}{K'} = d$ $\boxed{2}$ ✓

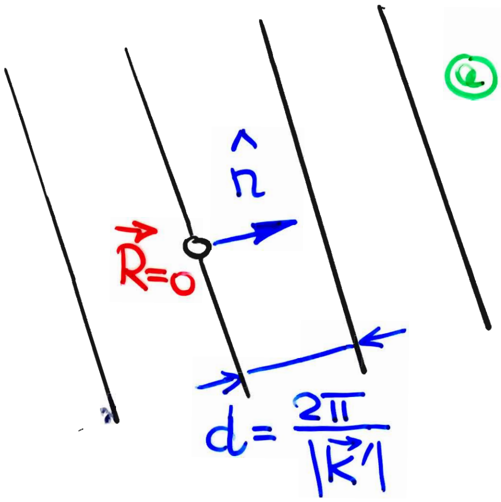
Theorem: Conversely

① $\forall \vec{K} \in RL$ determines a family of lattice planes $\perp \vec{K}$

② Distance between nearest planes

$$d = \frac{2\pi}{|\vec{K}'|}$$, where $\vec{K}'$ is the shortest RL $\parallel \hat{n} = \frac{\vec{K}}{|\vec{K}|}$

Proof: Consider $\vec{K}'$.



ⓐ A set of real space planes such that $e^{i\vec{K}'\cdot\vec{r}} = 1$ on them; $\vec{r}$ arbitrary otherwise.

ⓑ Since $\forall \vec{R} \in BL$ $e^{i\vec{K}'\cdot\vec{R}} = 1$

$\Rightarrow$ lattice planes lie among real space planes

ⓒ Spacing between lattice planes is $d = \frac{2\pi}{|\vec{K}'|}$. Suppose $d'' = \frac{2\pi}{|\vec{K}'|} \cdot N > d$.

Then $\vec{K}'' = \frac{1}{N}\vec{K}'$ would be a RL

But $|\vec{K}''| = \frac{|\vec{K}'|}{N} < |\vec{K}'|$

$|\vec{K}'|$ is the shortes

$\forall$ family of lattice planes $\Longleftrightarrow$ RL vector

$\hat{n}$, d $\qquad\qquad$ $\vec{K}' = \frac{2\pi}{d} \cdot \hat{n}$

direction, distance

Miller indices (hkl)

fix a set of RL primitive vectors

$\vec{b}_1, \vec{b}_2, \vec{b}_3$

$$\vec{K}' = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

- (hkl) integers $0, \pm 1, \pm 2, \ldots$
- $\vec{K}'$ is the shortest $\parallel \hat{n}$

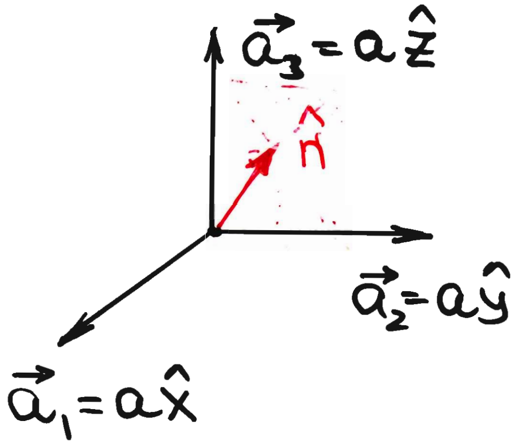
$\Rightarrow$ h, k, l don't have common factors

! **Note**: (hkl) depend on particular choice of primitive vectors $\vec{b}_1, \vec{b}_2, \vec{b}_3$ (and on $\vec{a}_1, \vec{a}_2, \vec{a}_3$ implicitly)

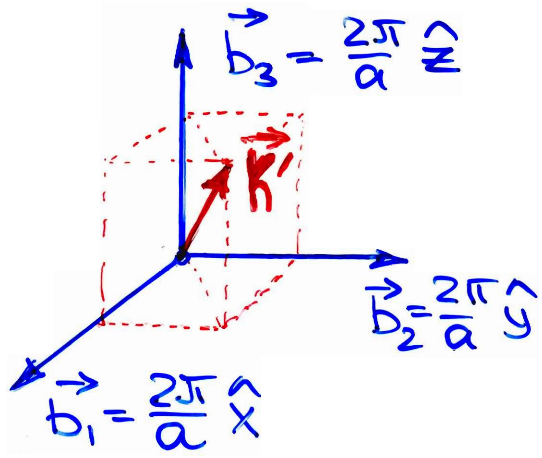
Important to understand – which primitive vectors are used!

In fact, very! important for non-cubic crystals

For simple cubic (SC) and (usual agreement) for BCC and FCC a conventional cubic cell is used



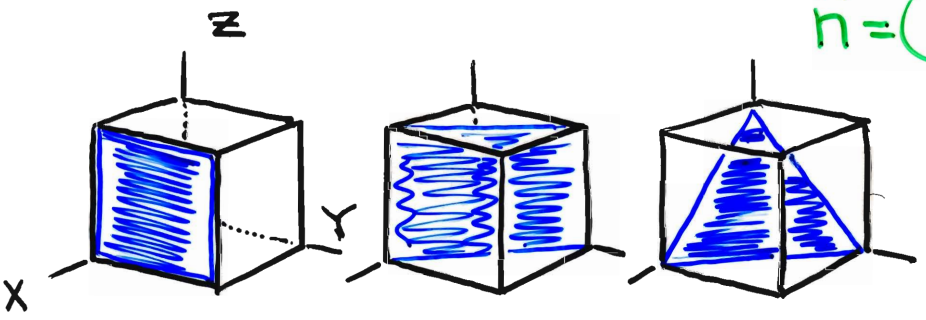
BL



RL

For cubic crystals (SC, BCC, FCC), Miller indices are [associated with] the coordinates of the normal to the plane $\hat{n}$

$\hat{n} = (1,0,0)$ $\hat{n} = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$ $\hat{n} = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$



(100) (110) (111)

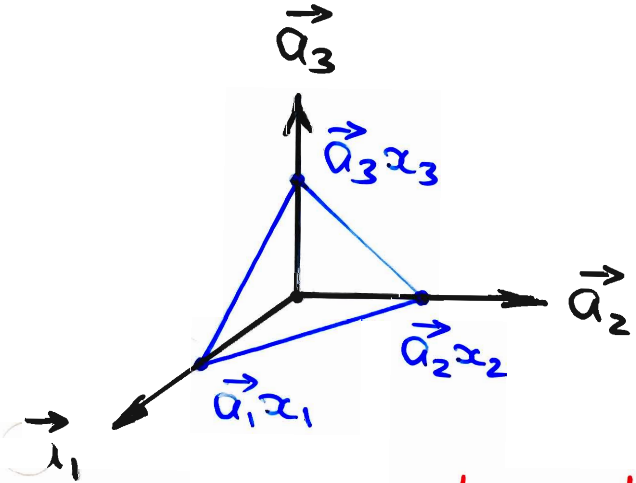
Another geometric interpretation of Miller indices $(hk\ell)$

A lattice plane $(hk\ell)$ $\perp$ $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$

$\Downarrow$

is contained in the continuous plane

$$\boxed{\vec{K}\cdot\vec{r} = A}$$ for suitable constant A



Intercepts satisfy

$\vec{K}\cdot\vec{a}_1 x_1 = A$

$\vec{K}\cdot\vec{a}_1 x_1 = h\vec{b}_1\cdot\vec{a}_1 x_1 = 2\pi h x_1$

$$\boxed{2\pi h x_1 = A}$$

$\vec{K}\cdot\vec{a}_2 x_2 = A$

$$\boxed{2\pi k x_2 = A}$$

$\vec{K}\cdot\vec{a}_3 x_3 = A$

$$\boxed{2\pi \ell x_3 = A}$$

$$\boxed{\begin{aligned} x_1 &= \frac{A}{2\pi h} \\ x_2 &= \frac{A}{2\pi k} \\ x_3 &= \frac{A}{2\pi \ell} \end{aligned}}$$

intercepts are $\Leftarrow$ inversely proportional to $(hk\ell)$

Another crystallographic definition of $(hk\ell)$:

① Determine intercepts x_1, x_2, x_3

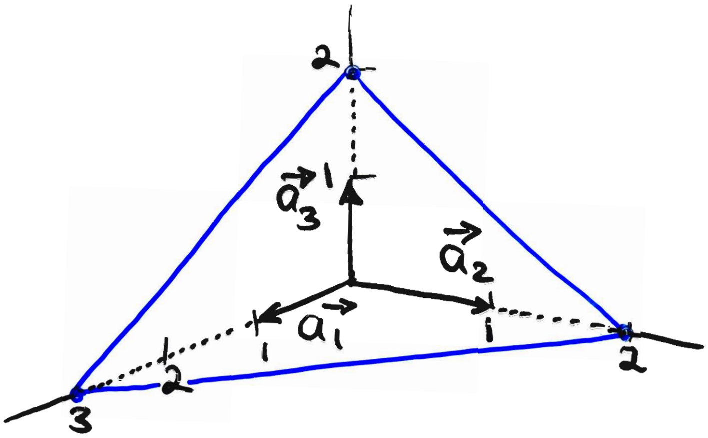
② Find integers with no common factors

$$h : k : \ell = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

4.6.1

Some examples

①

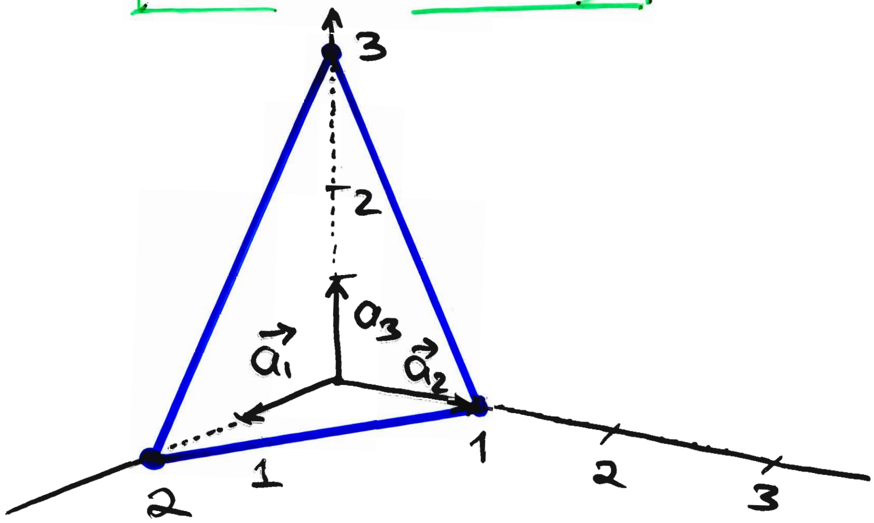


$x_1 = 3 \quad x_2 = 2 \quad x_3 = 2$

$h : k : l = \frac{1}{3} : \frac{1}{2} : \frac{1}{2}$ $\boxed{* 3 \cdot 2}$

$\boxed{(hkl) = (2\,3\,3)}$

②



$x_1 = 2 \quad x_2 = 1 \quad x_3 = 3$

$h : k : l = \frac{1}{2} : 1 : \frac{1}{3}$ $\boxed{* 3 \cdot 2}$

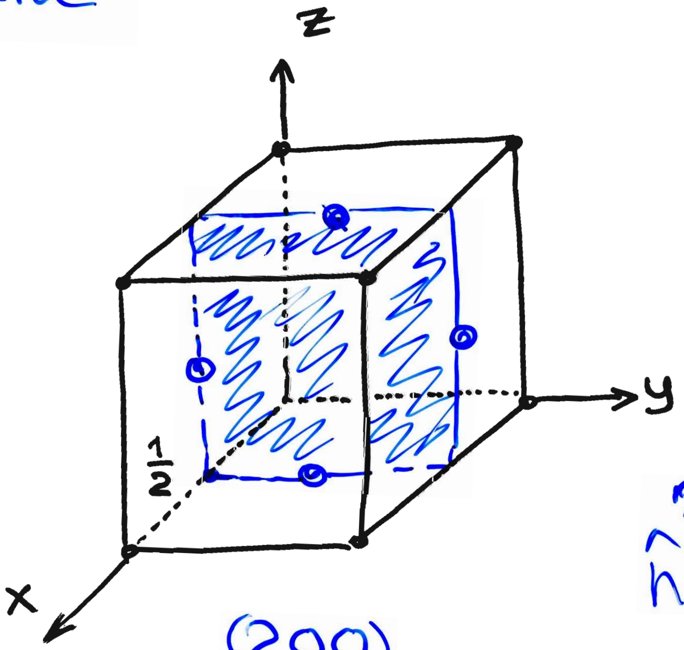
$\boxed{(hkl) = (3\,6\,2)}$

③ $x_1 = 3 \quad x_2 = 6 \quad x_3 = 7$

$h : k : l = \frac{1}{3} : \frac{1}{6} : \frac{1}{7}$ $\boxed{* 6 \cdot 7}$ $\boxed{(hkl) = (14\;7\;6)}$

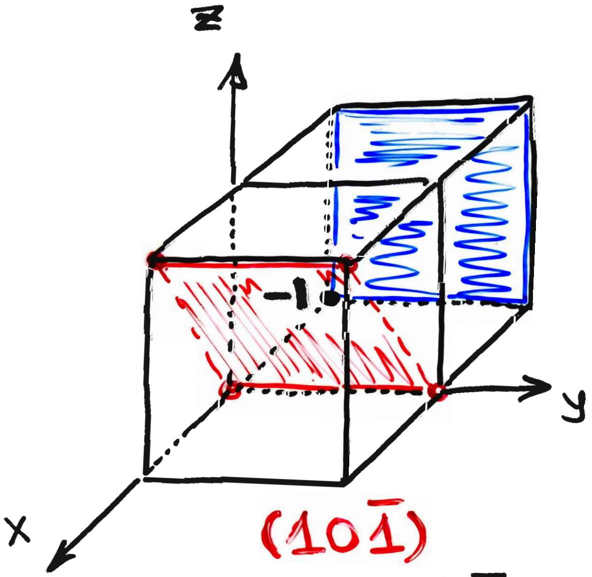
More examples

e.g.
FCC plane



(200)

$\hat{n} \overset{2}{=} \left(\frac{1}{2}, 0, 0\right)$

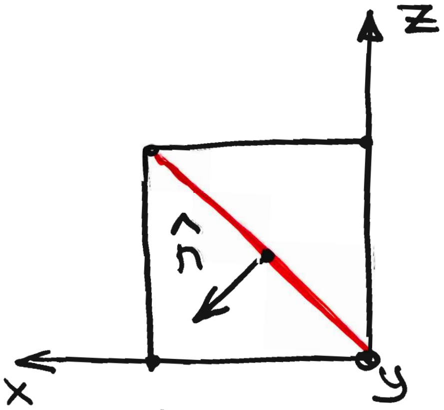


$(\bar{1}01)$

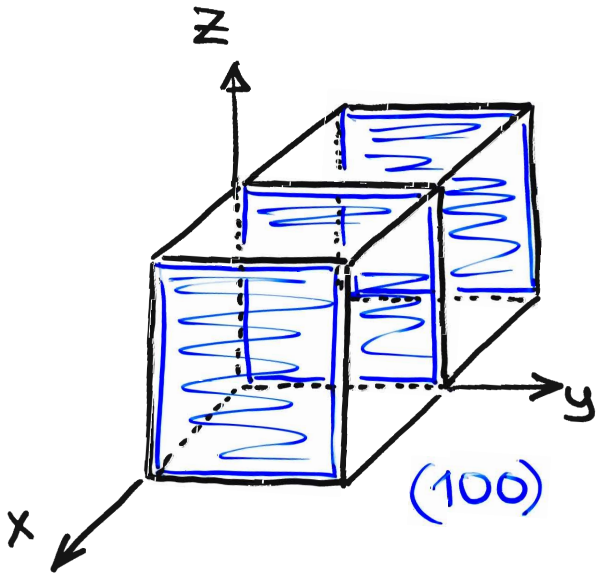
$(-100) \equiv (\bar{1}00)$

no commas
in notations

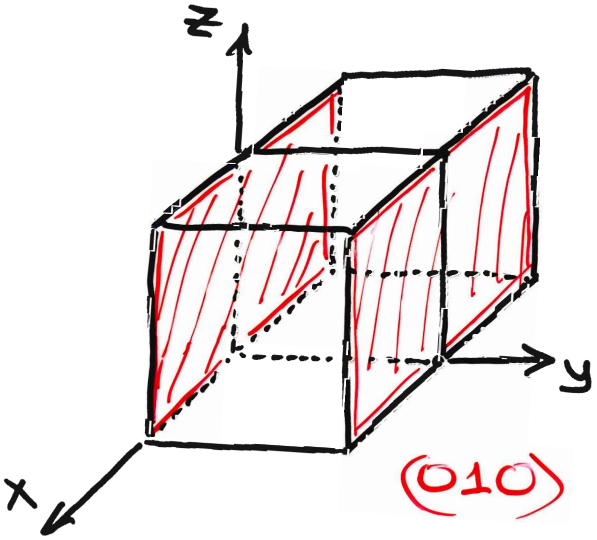
here (hkl) are used to identify a specific plane not just a family of (equivalent) planes



$\hat{n} = \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right) \Rightarrow (10-1) \equiv (10\bar{1})$



All Blue planes Belong to the same family (100)



Family of (010) planes

Due to cubic symmetry

(100) (010) (010) are physically equivalent

convention: {100} planes

{hkl} : (hkl) planes and all those that are equivalent to them by virtue of crystal symmetry

BRACES

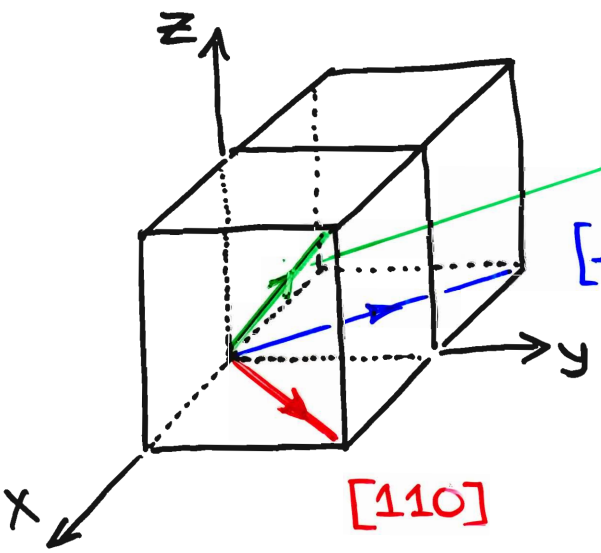
Directions in crystals

- Miller indices: defined using RL vectors $\vec{K}$ — (hkl) parenthesis

- We can directly specify directions in the direct BL — $[n_1 n_2 n_3]$ Brackets

Body diagonal: $[111]$

$[-1\,1\,0] \equiv [\bar{1}\,1\,0]$



Generally:
a lattice point $n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$
lies in the direction $[n_1 n_2 n_3]$

All Directions equivalent by virtue of the crystal symmetry: $\langle n_1 n_2 n_3 \rangle$

Example for cubic crystals:

$[110]$ $[\bar{1}10]$ $[\bar{1}\bar{1}0]$ $[1\bar{1}0]$

$[101]$ $[10\bar{1}]$ $[\bar{1}0\bar{1}]$ $[\bar{1}01]$

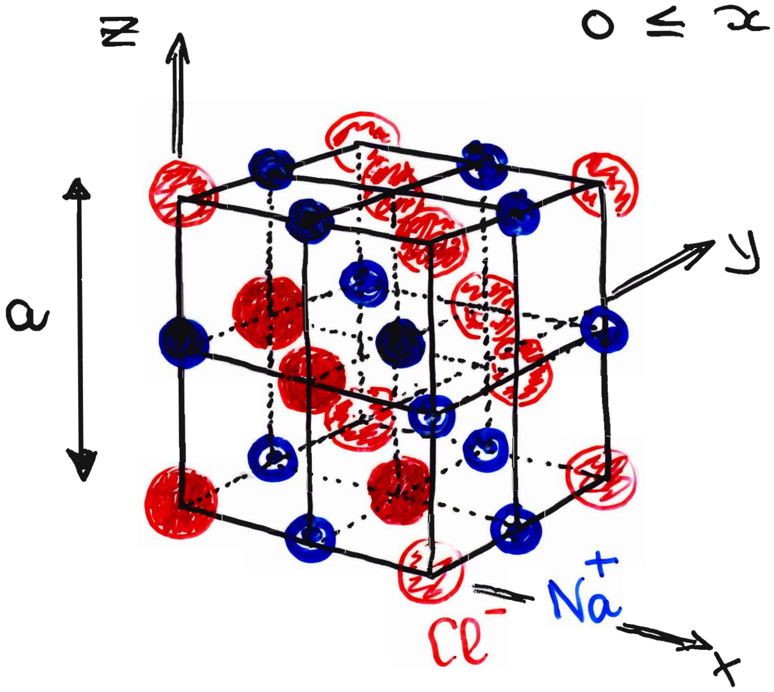
$\langle 110 \rangle$

$\boxed{\text{In cubic crystals the direction } [hkl] \text{ is perpendicular to a plane } (hkl)}$

A position of a point in a cell

$$\vec{r} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3$$

$$0 \le x_i \le 1$$



Sodium Chloride as an example

Considered as FCC with a Basis

Cl^-	000	$\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}0\frac{1}{2}$	$0\frac{1}{2}\frac{1}{2}$
Na^+	$00\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}01$	$0\frac{1}{2}1$