The reciprocal lattice

Outline

1. Definitions and properties
2. Important examples and applications
3. Miller indices of lattice planes

1. Definitions and properties
2. Important examples and applications
3. Miller indices of lattice planes

The reciprocal lattice

Definition

- Consider a set of points $\boldsymbol{R}$ constituting a Bravais lattice $\mathcal{R}$
- And a plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
  - $\boldsymbol{k}$: wave vector
  - planes orthogonal to $\boldsymbol{k}$ have the same phase (wave fronts)
- Reciprocal lattice: vectors $\boldsymbol{k}$ for which the plane wave has the periodicity of the Bravais lattice
  - the reciprocal lattice is defined w.r.t. a given Bravais lattice (direct lattice)
  - Lattice with a basis: consider only the underlying Bravais lattice

The reciprocal lattice

Definition

Mathematical definition

- $\boldsymbol{k}$ belongs to the reciprocal lattice if

$$e^{i\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{R})} = e^{i(\boldsymbol{k}\cdot\boldsymbol{r})} \qquad \forall \boldsymbol{R} \in \mathcal{R} \qquad \forall \boldsymbol{r} \in \mathbb{R}^3$$

- It follows that:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = 1 \longrightarrow \boldsymbol{k}\cdot\boldsymbol{R} = 2\pi n \qquad \forall \boldsymbol{R} \in \mathcal{R} \qquad n \in \mathbb{Z}$$

- We need to demonstrate that the set of vectors $\boldsymbol{k}$ constitute a lattice

The reciprocal lattice

The reciprocal lattice is a Bravais lattice

Demonstration/1

- The set of vectors $\{\mathbf{k}\}$ is closed under
- Addition:
  - If $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ belong to the r.l. also $\boldsymbol{k}_1 + \boldsymbol{k}_2$ belongs to the r.l.

$$e^{i(\boldsymbol{k}_1+\boldsymbol{k}_2)\cdot\boldsymbol{R}} = e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}} e^{i\boldsymbol{k}_2\cdot\boldsymbol{R}} = 1$$

- Subtraction:
  - If $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ belong to the r.l. also $\boldsymbol{k}_1 - \boldsymbol{k}_2$ belongs to the r.l.

$$e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{R}} = \frac{e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}}}{e^{i\boldsymbol{k}_2\cdot\boldsymbol{R}}} = 1$$

The reciprocal lattice

The reciprocal lattice is a Bravais lattice

Demonstration via explicit construction of the reciprocal lattice

- Given a set of primitive vectors of the Bravais lattice, $\{\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3\}$, define:

$$\begin{aligned} \boldsymbol{b}_1 &= 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \\ \boldsymbol{b}_2 &= 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \\ \boldsymbol{b}_3 &= 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)} \end{aligned}$$

- $V = \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$, the volume of the primitive cell
- $\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3) = \frac{(2\pi)^3}{V}$
- $\{\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3\}$ are a set of primitive vectors of the reciprocal lattice

The reciprocal lattice

The reciprocal lattice is a Bravais lattice

Demonstration via explicit construction of the reciprocal lattice

- The set $\{\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3\}$ is linearly independent if the $\{\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3\}$ is so
- The set $\{\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3\}$, satisfy $\boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij}$:
- Every wave vector $\boldsymbol{k}$ can be expressed as linear combination of $\boldsymbol{b}_i$:

$$\boldsymbol{k} = k_1\boldsymbol{b}_1 + k_2\boldsymbol{b}_2 + k_3\boldsymbol{b}_3$$

- For any vector $\boldsymbol{R}$ in the direct lattice, $\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$ we have:

$$\boldsymbol{k} \cdot \boldsymbol{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

- If $e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = 1$ then $\{k_1, k_2, k_3\}$ must be integers

The reciprocal lattice

The reciprocal of the reciprocal lattice

The reciprocal of the reciprocal lattice is the direct lattice: $(\mathcal{R}^*)^* = \mathcal{R}$

- Use the identity $\boldsymbol{A} \times (\boldsymbol{B} \times \boldsymbol{C}) = \boldsymbol{B}(\boldsymbol{A} \cdot \boldsymbol{C}) - \boldsymbol{C}(\boldsymbol{A} \cdot \boldsymbol{B})$

$$\begin{aligned}
\boldsymbol{c}_1 &= 2\pi \frac{\boldsymbol{b}_2 \times \boldsymbol{b}_3}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a}_1 \\
\boldsymbol{c}_2 &= 2\pi \frac{\boldsymbol{b}_3 \times \boldsymbol{b}_1}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a}_2 \\
\boldsymbol{c}_3 &= 2\pi \frac{\boldsymbol{b}_1 \times \boldsymbol{b}_2}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a}_3
\end{aligned}$$

- Alternatively:
  - Every wave vector $\boldsymbol{G} \in (\mathcal{R}^*)^*$ satisfies $e^{i\boldsymbol{G} \cdot \boldsymbol{K}} = 1$ for every $\boldsymbol{K}$
  - The direct lattice vectors $\boldsymbol{R}$ have already this property
  - Vectors not in the direct lattice have at least one non integer component

The reciprocal lattice

Cell volume of the reciprocal lattice

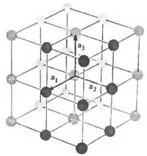
$V^* = \frac{(2\pi)^3}{V}$

- $V^* = \boldsymbol{b}_1 \cdot \boldsymbol{b}_2 \times \boldsymbol{b}_3$
- $\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3}$
- Vector identity: $(\boldsymbol{A} \times \boldsymbol{B}) \cdot (\boldsymbol{C} \times \boldsymbol{D}) = (\boldsymbol{A} \cdot \boldsymbol{C})(\boldsymbol{B} \cdot \boldsymbol{D}) - (\boldsymbol{A} \cdot \boldsymbol{D})(\boldsymbol{B} \cdot \boldsymbol{C})$
- 2D: $A^* = \frac{(2\pi)^2}{A}$
  - A is the area of the 2D primitive cell
- 1D: $a^* = \frac{2\pi}{a}$
  - a is the spacing btw lattice points of $\mathcal{R}$

Reciprocal lattice of selected Bravais lattices

SC Bravais lattice

- Consider a primitive cell of side a:
    - $\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}$, $\boldsymbol{a}_2 = a\hat{\boldsymbol{y}}$, $\boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$
- By definition:
    - $\boldsymbol{b}_1 = \frac{2\pi}{a}\hat{\boldsymbol{x}}$, $\boldsymbol{b}_2 = \frac{2\pi}{a}\hat{\boldsymbol{y}}$, $\boldsymbol{b}_3 = \frac{2\pi}{a}\hat{\boldsymbol{z}}$
- The reciprocal lattice is a simple cubic lattice with cubic primitive cell of side $\frac{2\pi}{a}$



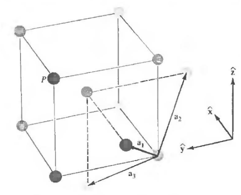
primitive vectors for a simple cubic Bravais lattice

Reciprocal lattice of selected Bravais lattices

FCC Bravais lattice

- The reciprocal lattice is described by a BCC conventional cell of side $\frac{4\pi}{a}$:

$$\begin{aligned}
\boldsymbol{b}_1 &= \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}} - \hat{\boldsymbol{x}}) \\
\boldsymbol{b}_2 &= \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}) \\
\boldsymbol{b}_3 &= \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}})
\end{aligned}$$



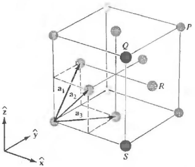
primitive vectors for the bcc Bravais lattice

Reciprocal lattice of selected Bravais lattices

BCC Bravais lattice

- The reciprocal lattice is described by a FCC conventional cell of side $\frac{4\pi}{a}$:

$$\begin{aligned} \boldsymbol{b}_1 &= \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}}) \\ \boldsymbol{b}_2 &= \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{z}}+\hat{\boldsymbol{x}}) \\ \boldsymbol{b}_3 &= \frac{4\pi}{a}\frac{1}{2}(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}) \end{aligned}$$

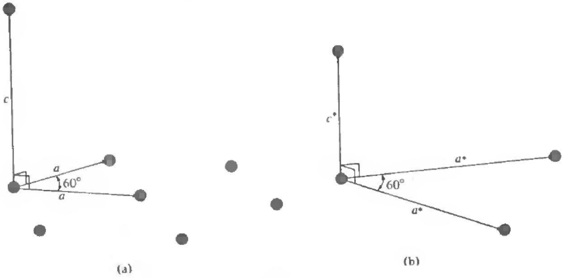


primitive vectors for the fcc Bravais lattice

Reciprocal lattice of selected Bravais lattices

Simple hexagonal Bravais lattice

- The reciprocal lattice is a simple hexagonal lattice
  - the lattice constants are $c^* = \frac{2\pi}{c}$, $a^* = \frac{4\pi}{\sqrt{3}a}$
  - rotated by 30° around the c axis w.r.t. the direct lattice

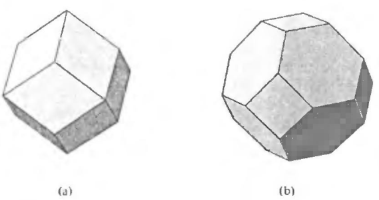


primitive vectors for (a) simple hexagonal Bravais lattice and (b) the reciprocal lattice

First Brillouin Zone

Definition

- The Wigner-Seitz cell of the reciprocal lattice
- Higher Brillouin zones arise in electronic structure theory
    - electronic levels in a periodic potential
- The terminology applies only to the reciprocal space (k-space)



first Brillouin zone for (a) bcc lattice and (b) fcc lattice

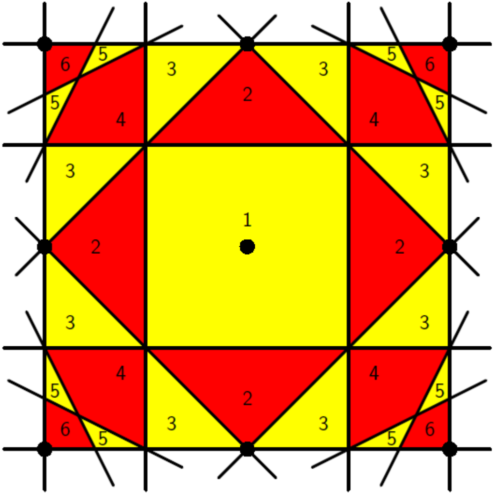
Higher Brillouin Zones

Brief intro

- 2nd, 3rd, . . . BZ are obtained with the same construction of the Wigner-Seitz cell:
  - connect the central points with lattice points around it
  - trace planes (lines in 2D) $\perp$ to the segments and intersecting at the mid point
- Regions of the reciprocal space are sorted based on volumes or areas (2D)
  - $V_1 < V_2 < V_3 \ldots$ or $A_1 < A_2 < A_3 \ldots$
- 2nd BZ: V_2 not including V_1
- 3nd BZ: V_3 not including V_1 and V_2
- and so on
  - Pictures of 2D higher BZ see web page of Ron Horgan ▸ Link

Higher Brillouin Zones

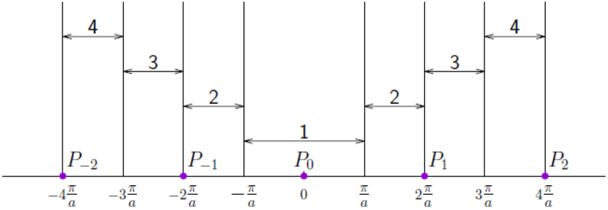
Brief intro



Higher Brillouin Zones

Brillouin zones for a 1D lattice

- 1st BZ: $[-\frac{\pi}{a}, \frac{\pi}{a}]$
- 2nd BZ: $[-\frac{2\pi}{a}, -\frac{\pi}{a}] \cup [\frac{\pi}{a}, \frac{2\pi}{a}]$
- 3rd BZ: $[-\frac{3\pi}{a}, -\frac{2\pi}{a}] \cup [\frac{2\pi}{a}, \frac{3\pi}{a}]$
- ...
- Boundaries are defined by $n\frac{\pi}{a}$, $n \in \mathbb{Z} \setminus 0$



Brillouin zones for a 1D lattice

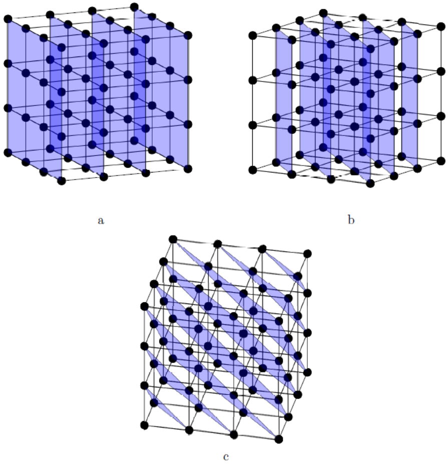
Lattice planes

Definition

- Any plane containing at least three non-collinear lattice points
- Any plane will contain infinitely many lattice points
    - translational symmetry of the lattice
    - 2D Bravais lattice within the plane
- Family of lattice planes:
    - all lattice planes that are parallel to a given lattice plane
    - the family contains all lattice points of the Bravais lattice
- The resolution of the Bravais lattice into a family of lattice planes is not unique

Lattice planes

Resolution of the Bravais lattice into a family of lattice planes



Three different resolutions of a simple cubic Bravais lattice into families of lattice planes

Lattice planes and reciprocal lattice vectors

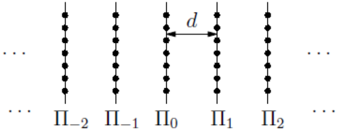
Theorem

- If d is the separation between lattice planes in a family, there are reciprocal lattice vectors $\perp$ to the planes, the shortest of which has a length $\frac{2\pi}{d}$. Conversely, $\forall \boldsymbol{k} \in \mathcal{R}^*$ there exists a family of lattice planes $\perp$ $\boldsymbol{k}$, separated by a distance d where $\frac{2\pi}{d}$ is the length of the shortest vector in the reciprocal space parallel to $\boldsymbol{k}$

Lattice planes and reciprocal lattice vectors

Proof $\Longrightarrow$

- Let $\mathcal{F}_\Pi$ be the family of lattice planes separated by d
  - Π_j, with $j \in \mathbb{Z}$ (Π_0 passes through the origin)
- Let $\hat{\boldsymbol{n}}$ be the normal to the planes
- $\boldsymbol{k} = \frac{2\pi}{d}\hat{\boldsymbol{n}}$ is a reciprocal lattice vector:
  - plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = c$ on planes $\perp \boldsymbol{k}$
  - has the same values on planes separated by $\lambda = \frac{2\pi}{k} = d$
  - $\mathcal{F}_\Pi$ is contained in its wave fronts
  - $e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = 1 \ \forall \boldsymbol{R} \in \Pi_0 \longrightarrow e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = 1 \ \forall \boldsymbol{R} \in \Pi_j,\ j \in \mathbb{Z}$

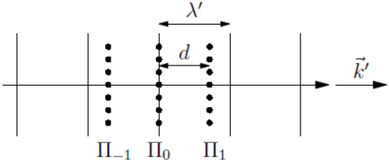


family of lattice planes $\mathcal{F}_\Pi$ separated by d

Lattice planes and reciprocal lattice vectors

Proof $\Longrightarrow$

- $\boldsymbol{k}$ is the shortest vector:
  - greater possible λ compatible with the spacing d of $\mathcal{F}_{\Pi}$
- Proved by reductio ad absurdum:
  - if $\exists \boldsymbol{k}' \in \mathcal{R}^*$, $\boldsymbol{k}' \parallel \boldsymbol{k} : k' = \frac{2\pi}{\lambda'} < k \longrightarrow \lambda' > d$
  - $\Pi_{\pm 1}$ are such that $e^{i\boldsymbol{k}'\cdot\boldsymbol{R}} \neq 1 \; \forall \boldsymbol{R} \in \Pi_{\pm 1}$
  - $\rightarrow \boldsymbol{k}' \notin \mathcal{R}^*$



Lattice planes and reciprocal lattice vectors

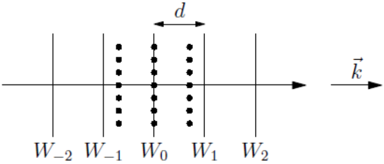
Proof $\Longleftarrow$

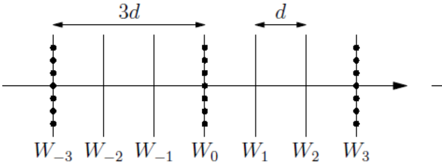
- Let $\boldsymbol{k} \in \mathcal{R}^*$ be the shortest reciprocal lattice vector
  - given a direction in $\mathcal{R}^*$
- Consider the set of real-space planes for which $e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = 1$
  - family $\mathcal{F}_{WF} = \{W_j : e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = 1 \quad \forall \boldsymbol{r} \in W_j \quad j \in \mathbb{Z}\}$
  - W_j's $\perp$ $\boldsymbol{k}$ (one contains the origin $\boldsymbol{r} = 0$)
  - W_j's are separated by $d = \frac{2\pi}{k}$
- $e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = 1 \ \forall \boldsymbol{R} \longrightarrow \mathcal{F}_{WF}$ must contain a family of lattice planes

Lattice planes and reciprocal lattice vectors

Proof $\Longleftarrow$

- The spacing must be d:
  - cannot be $d' < d$ (see figure below)
- cannot be $d' > d$, once again proved by reductio ad absurdum:
  - if $d' > d$ $\exists \boldsymbol{k}' \in \mathcal{R}^*$, $\boldsymbol{k}' \parallel \boldsymbol{k} : k' = \frac{2\pi}{d'} < k \longrightarrow \boldsymbol{k}$ is not the shortest reciprocal lattice vector





1. Definitions and properties

2. Important examples and applications

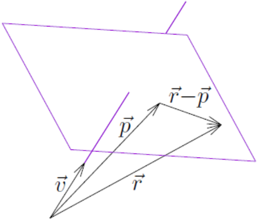
3. Miller indices of lattice planes

Miller indices of lattice planes

Correspondence between lattice planes and reciprocal lattice vectors

Equation of a plane

- The orientation is specified by giving a versor normal to the plane
- Let $\hat{\boldsymbol{v}} = (v_1, v_2, v_3)$ and a point $\boldsymbol{p} \in \Pi$, $\boldsymbol{p} = (p_1, p_2, p_3)$
- $\forall \boldsymbol{r} \in \Pi$: $\hat{\boldsymbol{v}} \cdot (\boldsymbol{r} - \boldsymbol{p}) = 0 \longrightarrow \hat{\boldsymbol{v}} \cdot \boldsymbol{r} = C$
- In cartesian components: $ax + by + cz = d$
    - $a = v_1,\ b = v_2,\ c = v_3,\ d = \hat{\boldsymbol{v}} \cdot \boldsymbol{p}$



$(\vec{r}-\vec{p})\cdot\vec{v}=0$

Miller indices of lattice planes

Correspondence between lattice planes and reciprocal lattice vectors

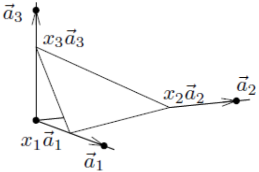
- A family of lattice planes can be specified by using $\boldsymbol{k} \in \mathcal{R}^*$ to specify the normal
    - use the vector of minimum modulus
- Miller indices of a plane: (hkl) components of the shortest $\boldsymbol{k} \in \mathcal{R}^* \perp$ to the plane
    - $\boldsymbol{k} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$
    - h, k, l are integers with no common factors
- Miller indices depend upon the choice of the primitive vectors of $\mathcal{R}^*$

Miller indices of lattice planes

Correspondence between lattice planes and reciprocal lattice vectors

Geometrical interpretation

- The plane is normal to the vector $\boldsymbol{k} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$
  - The equation of the plane is $\boldsymbol{k} \cdot \boldsymbol{r} = A$
  - Intersects $\{\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3\}$ at $\{x_1 = \frac{A}{2\pi h}, x_2 = \frac{A}{2\pi k}, x_3 = \frac{A}{2\pi l}\}$
- The intercepts are inversely proportional to the Miller indices of the plane.

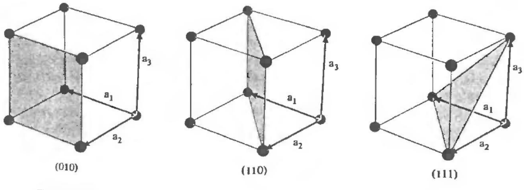


Crystallographic definition of the Miller indices, $h : k : l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$ or $x_1 : x_2 : x_3 = \frac{1}{h} : \frac{1}{k} : \frac{1}{l}$

Some conventions

Specification of lattice planes

- Simple cubic axes are used when the crystal has cubic symmetry
- A knowledge of the set of axis used is required
- Lattice planes are specified by giving the Miller indices *(hkl)*
  - Plane with a normal vector (4,-2,1) $\Longrightarrow$ $(4\bar{2}1)$
- Planes equivalent by virtue of the crystal symmetry:
  - (100),(010), and (001) are equivalent in cubic crystals
  - collectively referred to as $\{100\}$ planes ($\{hkl\}$ planes in general)

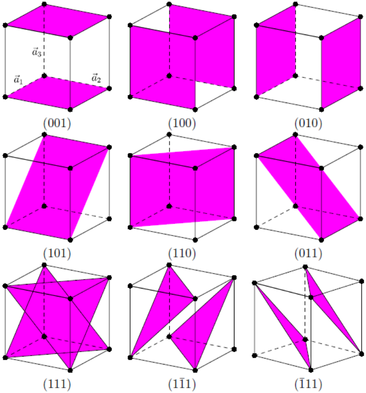


(010) (110) (111)

Lattice planes and Miller indices in a simple cubic Bravais lattice

Some conventions

Example of lattice planes and corresponding Miller indices



Some conventions

Specification of directions in the direct lattice

- The lattice point $n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$ lies in the $[n_1 n_2 n_3]$ direction
  - from the origin
- Directions equivalent by virtue of the crystal symmetry:
  - $[100]$, $[\bar{1}00]$,$[010]$,$[0\bar{1}0]$,$[001]$,$[00\bar{1}]$ are equivalent in cubic crystals
  - collectively referred to as $< 100 >$ directions