The reciprocal lattice

Outline

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
- and a plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
  - $\boldsymbol{k}$: wave vector
  - Planes orthogonal to $\boldsymbol{k}$ have the same phase
- Reciprocal lattice: Values of $\boldsymbol{k}$ 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

$$e^{i\boldsymbol{K}\cdot(\boldsymbol{r}+\boldsymbol{R})} = e^{i(\boldsymbol{k}\cdot\boldsymbol{r})}$$

  - For every lattice vector $\boldsymbol{R}$ of the Bravais lattice
- It follows that

$$e^{i\boldsymbol{K}\cdot\boldsymbol{R}} = 1$$

- 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 $\boldsymbol{b}_i \cdot \boldsymbol{a_j} = \delta_{ij}$:
- 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

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

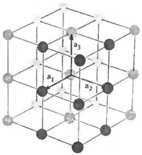
$$\begin{aligned}
\boldsymbol{c}_1 &= 2\pi \frac{\boldsymbol{b}_2 \times \boldsymbol{b}_3}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a_1} \\
\boldsymbol{c}_2 &= 2\pi \frac{\boldsymbol{b}_3 \times \boldsymbol{b}_1}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a_2} \\
\boldsymbol{c}_3 &= 2\pi \frac{\boldsymbol{b}_1 \times \boldsymbol{b}_2}{\boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3)} = \boldsymbol{a_3}
\end{aligned}$$

- Alternatively:
  - Every wave vector $\boldsymbol{G}$ that satisfy $e^{i\boldsymbol{G}\cdot\boldsymbol{K}} = 1$ 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

Reciprocal lattice of selected Bravais lattices

Simple cubic

- Consider a primitive cell of side a:
  - $\boldsymbol{a}_1 = a\hat{\boldsymbol{x}}$, $\boldsymbol{a}_2 = a\hat{\boldsymbol{y}}$, $\boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$
- Then, 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 $\frac{2\pi}{a}$



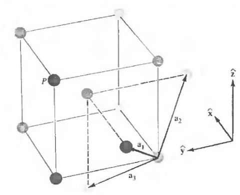
Primitive vectors for a simple cubic Bravais lattice

Reciprocal lattice of selected Bravais lattices

Face centered cubic

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

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



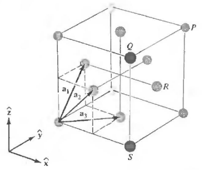
Primitive vectors for the bcc Bravais lattice

Reciprocal lattice of selected Bravais lattices

Body centered cubic

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

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

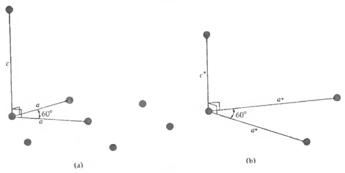


Primitive vectors for the fcc Bravais lattice

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

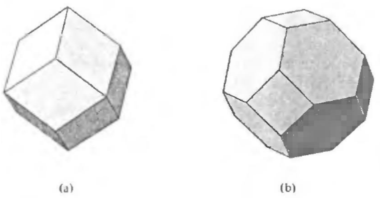


Primitive vectors for (a) simple hexagonal Bravais lattice and (b) the reciprocal lattice

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 apply only to the reciprocal space (k-space)

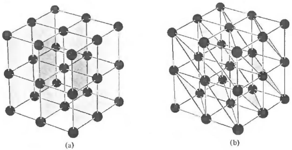


First Brillouin zone for (a) bcc lattice and (b) fcc lattice

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



Two 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, $\forall \boldsymbol{K}$ 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 $\hat{\boldsymbol{n}}$ be the normal to the planes
- $\boldsymbol{K} = \frac{2\pi}{d}\hat{\boldsymbol{n}}$ is a reciprocal lattice vector:
  - $e^{i\boldsymbol{K}\cdot\boldsymbol{r}} = c$ on planes $\perp$ $\boldsymbol{K}$
  - Has the same values on planes separated by $\lambda = \frac{2\pi}{K} = d$
  - $e^{i\boldsymbol{K}\cdot\boldsymbol{r}} = 1$ for the plane passing through the origin ($\boldsymbol{r} = 0$)
  - $e^{i\boldsymbol{K}\cdot\boldsymbol{R}} = 1$ for any lattice point
  - $\boldsymbol{K}$ is the shortest vector (greater possible wavelength compatible with the spacing d)

Lattice planes and reciprocal lattice vectors

Proof $\Longleftarrow$

- Let $\boldsymbol{K}$ be the shortest parallel reciprocal lattice vector (given a vector in the reciprocal space)
- Consider the set of real-space planes for which $e^{i\boldsymbol{K}\cdot\boldsymbol{r}} = 1$
  - all planes are $\perp$ $\boldsymbol{K}$ (one contains the origin $\boldsymbol{r} = 0$)
  - they are separated by $d = \frac{2\pi}{K}$
- Since $e^{i\boldsymbol{K}\cdot\boldsymbol{R}} = 1 \ \forall\boldsymbol{R}$, the set of planes must contain a family of planes
- The spacing must be d
  - Otherwise $\boldsymbol{K}$ would not be the shortest reciprocal lattice vector (reductio ad absurdum)

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

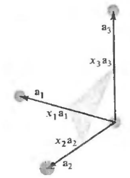
- The orientation of a plane is specified by giving a vector normal to the plane
- We can use reciprocal lattice vectors to specify the normal
    - use the shortest vector
- Miller indices of a plane (hkl): components of the shortest reciprocal lattice vector ⊥ to the plane
    - $h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$
    - h, k, l are integers with no common factors
- The Miller indices depend on the choice of the primitive vectors

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 $\boldsymbol{K} \cdot \boldsymbol{r} = A$
  - Intersect the primitive vectors $\{\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3\}$ at $\{x_1 = \frac{A}{2\pi h}, x_2 = \frac{A}{2\pi k}, x_3 = \frac{A}{2\pi l}\}$
- The intercepts with the crystal axis are inversely proportional to the Miller indices of the plane.

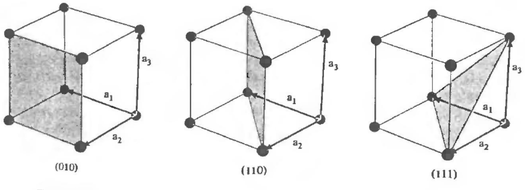


Crystallographic definition of the Miller indices, $h : k : l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$

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)



Lattice planes and Miller indices in a simple cubic Bravais lattice

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