Reciprocal lattice

Wikipedia, 09/14/07

In crystallography, the **reciprocal lattice** of a Bravais lattice is the set of all vectors **K** such that

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

for all lattice point position vectors **R**. The reciprocal lattice is itself a Bravais lattice, and the reciprocal of the reciprocal lattice is the original lattice.

For a three dimensional lattice, defined by its primitive vectors $(\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3})$, its reciprocal lattice can be determined by generating its three reciprocal primitive vectors, through the formula,

$$\mathbf{b_1} = 2\pi \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})}$$

$$\mathbf{b_2} = 2\pi \frac{\mathbf{a_3} \times \mathbf{a_1}}{\mathbf{a_2} \cdot (\mathbf{a_3} \times \mathbf{a_1})}$$

$$\mathbf{b_3} = 2\pi \frac{\mathbf{a_1} \times \mathbf{a_2}}{\mathbf{a_3} \cdot (\mathbf{a_1} \times \mathbf{a_2})}$$

Using column vector representation of (reciprocal) primitive vectors, the formula above can be rewritten using matrix inversion:

$$\left[\mathbf{b_1}\mathbf{b_2}\mathbf{b_3}\right]^T = 2\pi \left[\mathbf{a_1}\mathbf{a_2}\mathbf{a_3}\right]^{-1}$$

This method appeals to the definition, and allows generalization to arbitrary dimensions. Curiously, the cross product formula dominates introductory materials on crystallography.

The above definition is called the "physics" definition, as the factor of 2π comes naturally from the study of periodic structures. An equivalent definition, the "crystallographer's" definition, comes from defining the reciprocal lattice to be $e^{2\pi i\mathbf{K}\cdot\mathbf{R}} = 1$ which changes the definitions of the reciprocal lattice vectors to be

$$\mathbf{b_1} = \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})}$$

and so on for the other vectors. The crystallographer's definition has the advantage that the definition of $\mathbf{b_1}$ is just the reciprocal magnitude of $\mathbf{a_1}$ in the direction of $\mathbf{a_2} \times \mathbf{a_3}$, dropping the factor of 2π; this can simplify certain mathematical manipulations. It is a matter of taste which definition of the lattice is used, as long as the two are not mixed.

Each point (hkl) in the reciprocal lattice corresponds to a set of lattice planes (hkl) in the real space lattice. The direction of the reciprocal lattice vector corresponds to the normal to the real space planes, and the magnitude of the reciprocal lattice vector is equal to the reciprocal of the interplanar spacing of the real space planes.

The reciprocal lattice plays a fundamental role in most analytic studies of periodic structures, particularly in the theory of diffraction. For Bragg reflections in neutron and X-ray diffraction, the momentum difference between incoming and diffracted X-rays of a crystal is a reciprocal lattice vector. The diffraction pattern of a crystal can be used to determine the reciprocal vectors of the lattice. Using this process, one can infer the atomic arrangement of a crystal.

The Brillouin zone is a primitive unit cell of the reciprocal lattice.

Reciprocal lattices of various crystals

Reciprocal lattices for the cubic crystal system are as follows.

Simple cubic lattice

We find that the simple cubic Bravais lattice, with cubic primitive cell of side *a*, has for its reciprocal a simple cubic lattice with a cubic primitive cell of side $\frac{2\pi}{a}$ ($\frac{1}{a}$ in the crystallographer's definition). The cubic lattice is therefore said to be dual, having its reciprocal lattice being identical (up to a numerical factor).

Face-centered cubic lattice

The reciprocal lattice to an FCC lattice is the BCC lattice.

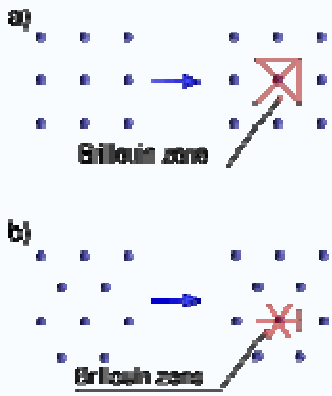
Body-centered cubic lattice

The reciprocal lattice to an BCC lattice is the FCC lattice.

It can be easily proven that only the Bravais lattices which have 90 degrees between $(\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3})$(cubic, tetragonal, orthorhombic) have $(\mathbf{b_1}, \mathbf{b_2}, \mathbf{b_3})$ parallel to their real-space vectors.

Brillouin Zones

Wikipedia, 09/14/07



Brillouin zone

In mathematics and solid state physics, the first **Brillouin zone** is a uniquely defined primitive cell of the reciprocal lattice in the frequency domain. It is found by the same method as for the Wigner-Seitz cell in the Bravais lattice. The importance of the Brillouin zone stems from the Bloch wave description of waves in a periodic medium, in which it is found that the solutions can be completely characterized by their behavior in a single Brillouin zone.

Taking the surfaces at the same distance from one element of the lattice and its neighbours, the volume included is the first Brillouin zone. Another definition is as the set of points in *k*-space that can be reached from the origin without crossing any Bragg plane.

There are also second, third, *etc.*, Brillouin zones, corresponding to a sequence of disjoint regions (all with the same volume) at increasing distances from the origin, but these are used more rarely. As a result, the *first* Brillouin zone is often called simply the *Brillouin zone*. (In general, the n-th Brillouin zone consist of the set of points that can be reached from the origin by crossing $n - 1$ Bragg planes.)

A related concept is that of the **irreducible Brillouin zone**, which is the first Brillouin zone reduced by all of the symmetries in the point group of the lattice.

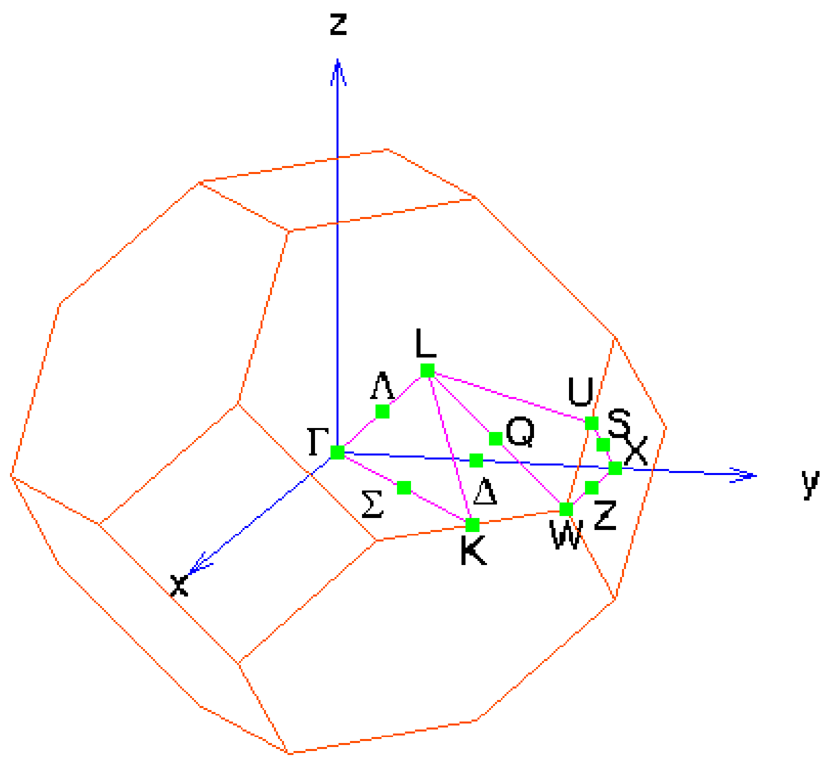
The concept of a Brillouin zone was developed by Leon Brillouin(1889-1969), a French physicist.

Critical points

Several points of high symmetry are of special interest – these are called critical points.[1]

Symbol	Description
Γ	Center of the Brillouin zone
Simple cube	
M	Center of an edge
R	Corner point
X	Center of a face
Face-centered cubic	
K	Middle of an edge joining two hexagonal faces
L	Center of a hexagonal face
U	Middle of an edge joining a hexagonal and a square face
W	Corner point
X	Center of a square face
Body-centered cubic	
H	Corner point joining four edges
N	Center of a face
P	Corner point joining three edges
Hexagonal	
A	Center of a hexagonal face
H	Corner point
K	Middle of an edge joining two rectangular faces
L	Middle of an edge joining a hexagonal and a rectangular face
M	Center of a rectangular face

Brillouin zone for the fcc unit cell



Label	Cartesian Coordinates	Lattice Coordinates	Range
Γ	(0 , 0 , 0)	0	Point
Δ	(0 , 2 π x/a , 0)	½ x ($\mathbf{b}_1$ + $\mathbf{b}_3$)	0 < x < 1
X	(0 , 2 π/a , 0)	½ ($\mathbf{b}_1$ + $\mathbf{b}_3$)	Point
Z	(½ x π/a , 2 π/a , 0)	½ $\mathbf{b}_1$ + ¼ x $\mathbf{b}_2$ + ¼ (2+x) $\mathbf{b}_3$	0 < x < 1
W	(π/a , 2 π/a , 0)	½ $\mathbf{b}_1$ + ¼ $\mathbf{b}_2$ + ¾ $\mathbf{b}_3$	Point
Q	(π/a , (2 - x) π/a , x π/a)	½ $\mathbf{b}_1$ + ¼ (1 + x) $\mathbf{b}_2$ + ¼ (3 - x) $\mathbf{b}_3$	0 < x < 1
L	(π/a , π/a , π/a)	½ $\mathbf{b}_1$ + ½ $\mathbf{b}_2$ + ½ $\mathbf{b}_3$	Point
Λ	(x π/a , x π/a , x π/a)	½ x $\mathbf{b}_1$ + ½ x $\mathbf{b}_2$ + ½ x $\mathbf{b}_3$	0 < x < 2
Σ	(2 π x/a , 2 π x/a , 0)	½ x $\mathbf{b}_1$ + ½ x $\mathbf{b}_2$ + x $\mathbf{b}_3$	0 < x < ¾
K = U	($^3/_2$ π/a , $^3/_2$ π/a , 0)	$^3/_8$ $\mathbf{b}_1$ + $^3/_8$ $\mathbf{b}_2$ + ¾ $\mathbf{b}_3$	Point
S	(2 π x/a , 2 π x/a , 0)	½ x $\mathbf{b}_1$ + ½ x $\mathbf{b}_2$ + x $\mathbf{b}_3$	¾ < x < 1
X'	(2 π/a , 2 π/a , 0)	½ $\mathbf{b}_1$ + ½ $\mathbf{b}_2$ + $\mathbf{b}_3$	Point

Brillouin zone for the hcp unit cell