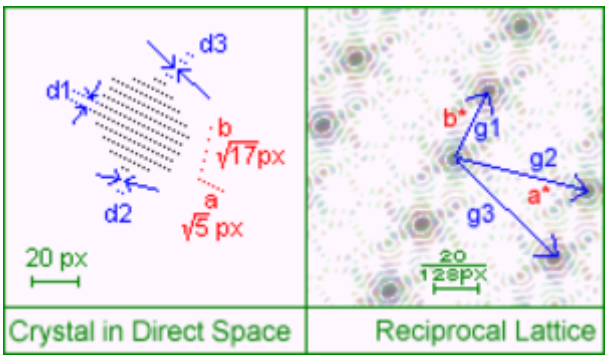
# Reciprocal lattice

In physics, the **reciprocal lattice** represents the Fourier transform of another lattice (usually a Bravais lattice). In normal usage, this first lattice (whose transform is represented by the reciprocal lattice) is usually a periodic spatial function in real-space and is also known as the *direct lattice*. While the direct lattice exists in real-space and is what one would commonly understand as a physical lattice, the reciprocal lattice exists in reciprocal space (also known as *momentum space* or less commonly as *K-space*, due to the relationship between the Pontryagin duals momentum and position.) The reciprocal lattice of a reciprocal lattice, then, is the original direct lattice again, since the two lattices are Fourier transforms of each other



A two-dimensional crystal and its reciprocal lattice

The reciprocal lattice plays a fundamental role in most analytic studies of periodic structures, particularly in the theory of diffraction. In neutron and X-ray diffraction, due to the Laue conditions, 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 Wigner-Seitz cell of the reciprocal lattice.

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## Mathematical description

Assuming a two-dimensionalBravais lattice

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 \text{ where } n_1, n_2 \in \mathbb{Z}.$$

Any quantity, e.g. the electronic density in an atomic crystal can be written as a periodic function

$$f(\mathbf{r}) = f(\mathbf{R_n} + \mathbf{r})$$

Due to the periodicity, it is useful to write $f$ as a Fourier series

$$f\left(\mathbf{R}_n + \mathbf{r}\right) = \sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} e^{i\mathbf{G}_m \cdot \mathbf{R}_n}$$

Since $f(\mathbf{R}_n + \mathbf{r}) = f\left(\mathbf{R}_k + \mathbf{r}\right)$ for any $n, k \in \mathbb{Z}^2$ then the last formula is true for the particular case $\mathbf{R}_0 = 0$

$$\sum_m f_m \left(e^{i\mathbf{G}_m \cdot \mathbf{r}}\right)\left(e^{i\mathbf{G}_m \cdot \mathbf{R}_n}\right) = \sum_m f_m \left(e^{i\mathbf{G}_m \cdot \mathbf{r}}\right)\left(e^{i\mathbf{G}_m \cdot 0}\right) = \sum_m f_m \left(e^{i\mathbf{G}_m \cdot \mathbf{r}}\right) (1)$$

so must be true $e^{i\mathbf{G}_m \cdot \mathbf{R}_n} = 1$ that means

$$\mathbf{G}_m \cdot \mathbf{R}_n = 2\pi N \text{ where } N \in \mathbb{Z}.$$

Mathematically, we can describe the reciprocal lattice as the set of all vectors $\mathbf{G}_m$ that satisfy the above identity for all lattice point position vectors $\mathbf{R}$.

This reciprocal lattice is itself a Bravais lattice, and the reciprocal of the reciprocal lattice is the original lattice, which reveals the Pontryagin duality of their respective vector spaces.

For an infinite two-dimensional lattice, defined by its primitive vectors $(\mathbf{a_1}, \mathbf{a_2})$, its reciprocal lattice can be determined by generating its two reciprocal primitive vectors, through the following formulae,

$$\mathbf{G}_m = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2$$

Where,

$$\mathbf{b}_1 = 2\pi \frac{-\mathbf{R}\,\mathbf{a}_2}{-\mathbf{a}_1 \cdot \mathbf{R}\,\mathbf{a}_2} = 2\pi \frac{\mathbf{R}\,\mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{R}\,\mathbf{a}_2}$$
$$\mathbf{b}_2 = 2\pi \frac{\mathbf{R}\,\mathbf{a}_1}{\mathbf{a}_2 \cdot \mathbf{R}\,\mathbf{a}_1}$$

Here $\mathbf{R}$ represents a 90 degree rotation matrix.

For an infinite 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 formulae

$$\mathbf{G}_m = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3$$

where

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

Note that the denominator is the scalar triple product. Using column vector representation of (reciprocal) primitive vectors, the formulae above can be rewritten using matrix inversion:

$$[\mathbf{b}_1\,\mathbf{b}_2\,\mathbf{b}_3]^{\mathsf{T}} = 2\pi [\mathbf{a}_1\,\mathbf{a}_2\,\mathbf{a}_3]^{-1}.$$

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

The above definition is called the "physics" definition, as the factor of $2\pi$ 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 $2\pi$. This can simplify certain mathematical manipulations, and expresses reciprocal lattice dimensions in units of spatial frequency. 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. The magnitude of the reciprocal lattice vector is given in reciprocal length and is equal to the reciprocal of the interplanar spacing of the real space planes.

# Reciprocal lattices of various crystals

Reciprocal lattices for the cubic crystal system are as follows.

## Simple cubic lattice

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 self-dual, having the same symmetry in reciprocal space as in real space.

## Face-centered cubic (FCC) lattice

The reciprocal lattice to an FCC lattice is the body-centered cubic (BCC) lattice.

Consider an FCC compound unit cell. Locate a primitive unit cell of the FCC; i.e., a unit cell with one lattice point. Now take one of the vertices of the primitive unit cell as the origin. Give the basis vectors of the real lattice. Then from the known formulae, you can calculate the basis vectors of the reciprocal lattice. These reciprocal lattice vectors of the FCC represent the basis vectors of a BCC real lattice. Note that the basis vectors of a real BCC lattice and the reciprocal lattice of an FCC resemble each other in direction but not in magnitude.

## Body-centered cubic (BCC) lattice

The reciprocal lattice to a 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.

## Simple hexagonal lattice

The reciprocal to a simple hexagonal Bravais lattice with lattice constants c and a is another simple hexagonal lattice with lattice constants $\frac{2\pi}{c}$ and $\frac{4\pi}{a\sqrt{3}}$ rotated through 30° about the c axis with respect to the direct lattice. The simple hexagonal lattice is therefore said to be self-dual, having the same symmetry in reciprocal space as in real space.

### Proof that the reciprocal lattice of the reciprocal lattice is the direct lattice

From its definition we know that the vectors of the Bravais lattice must be closed under vector addition and subtraction. Thus it is sufficient to say that if we have

$$e^{i\mathbf{G}_1 \cdot \mathbf{R}} = 1$$

and

$$e^{i\mathbf{G}_2 \cdot \mathbf{R}} = 1$$

then the sum and difference $\mathbf{G}_1 \pm \mathbf{G}_2$ satisfy the same.

$$e^{i(\mathbf{G}_1 + \mathbf{G}_2)\mathbf{R}} = \left(e^{i\mathbf{G}_1 \cdot \mathbf{R}}\right)\left(e^{i\mathbf{G}_2 \cdot \mathbf{R}}\right) = (1)(1) = 1$$
$$e^{i(\mathbf{G}_1 - \mathbf{G}_2)\cdot \mathbf{R}} = \frac{e^{i\mathbf{G}_1 \cdot \mathbf{R}}}{e^{i\mathbf{G}_2 \cdot \mathbf{R}}} = 1$$

Thus we have shown the reciprocal lattice is closed under vector addition and subtraction. Furthermore, we know that a vector **G** in the reciprocal lattice can be expressed as a linear combination of its primitive vectors

$$\mathbf{G} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$$

From our earlier definition of $\mathbf{b}_1$, we can see that:

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

where $\delta_{ij}$ is the Kronecker delta. We let **R** be a vector in the direct lattice, which we can express as a linear combination of *its* primitive vectors.

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

From this we can see that:

$$\mathbf{G} \cdot \mathbf{R} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3)$$

From our definition of the reciprocal lattice we have shown that $\mathbf{G}$ must satisfy the following identity

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

For this to hold we must have $\mathbf{G} \cdot \mathbf{R}$ equal to $2\pi$ times an integer. This is fulfilled because $n_i \in \mathbb{Z}$ and $k_i \in \mathbb{Z}$. Therefore, the reciprocal lattice is also a Bravais lattice.

Furthermore, if the vectors $\mathbf{G}$ construct a reciprocal lattice, it is clear that any vector $\mathbf{K}$ satisfying the equation:

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

… is a reciprocal lattice vector of the reciprocal lattice. Due to the definition of $\mathbf{G}$, when $\mathbf{K}$ is the direct lattice vector $\mathbf{R}$, we have the same relationship.

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

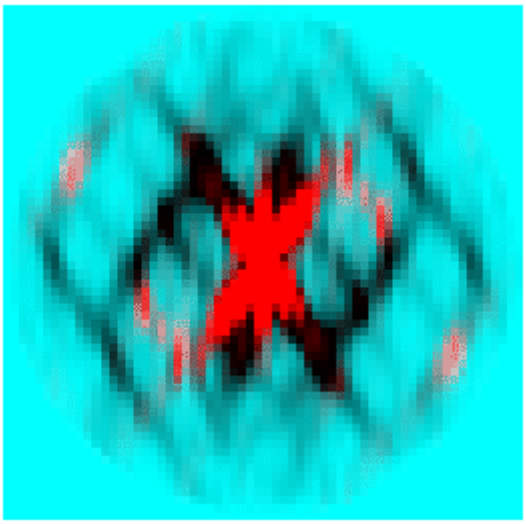
And so we can conclude that the reciprocal lattice of the reciprocal lattice is the original direct lattice.

# Arbitrary collection of atoms

One path to the reciprocal lattice of an arbitrary collection of atoms comes from the idea of scattered waves in the Fraunhofer (long-distance or lens back-focal-plane) limit as a Huygens-style sum of amplitudes from all points of scattering (in this case from each individual atom).[1] This sum is denoted by the complex amplitude F in the equation below, because it is also the Fourier transform (as a function of spatial frequency or reciprocal distance) of an effective scattering potential in direct space:

$$F[\vec{g}] = \sum_{j=1}^{N} f_j\,[\vec{g}]\; e^{2\pi i \vec{g}\cdot\vec{r}_j}.$$

Here **g** = **q**/(2π) is the scattering vector **q** in crystallographer units, N is the number of atoms, $f_j[\mathbf{g}]$ is the atomic scattering factor for atom j and scattering vector **g**, while $\mathbf{r}_j$ is the vector position of atom j. Note that the Fourier phase depends on one's choice of coordinate origin.



Shadow of a 118-atom faceted carbon-pentacone's intensity reciprocal-lattice lighting up red in diffraction when intersecting the Ewald sphere.

For the special case of an infinite periodic crystal, the scattered amplitude F = M $F_{hkl}$ from M unit cells (as in the cases above) turns out to be non-zero only for integer values of $(hkl)$, where

$$F_{hkl} = \sum_{j=1}^{m} f_j\,[g_{hkl}]\; e^{2\pi i(hu_j + kv_j + lw_j)}$$

when there are j=1,m atoms inside the unit cell whose fractional lattice indices are respectively $\{u_j, v_j, w_j\}$. To consider effects due to finite crystal size, of course, a shape convolution for each point or the equation above for a finite lattice must be used instead.

Whether the array of atoms is finite or infinite, one can also imagine an "intensity reciprocal lattice" I[**g**], which relates to the amplitude lattice F via the usual relation $I = F^*F$ where $F^*$ is the complex conjugate of F. Since Fourier transformation is reversible, of course, this act of conversion to intensity tosses out "all except 2nd moment" (i.e. the phase) information. For the case of an arbitrary collection of atoms, the intensity reciprocal lattice is therefore:

$$I[\vec{g}] = \sum_{j=1}^{N}\sum_{k=1}^{N} f_j\,[\vec{g}]\; f_k\,[\vec{g}]\; e^{2\pi i \vec{g}\cdot\vec{r}_{jk}}.$$

Here $\mathbf{r}_{jk}$ is the vector separation between atom j and atom k. One can also use this to predict the effect of nano-crystallite shape, and subtle changes in beam orientation, on detected diffraction peaks even if in some directions the cluster is only one atom thick. On the down side, scattering calculations using the reciprocal lattice basically consider an incident plane wave. Thus after a first look at reciprocal lattice (kinematic scattering) effects, beam broadening and multiple scattering (i.e. dynamical) effects may be important to consider as well.

# Generalization of a dual lattice

There are actually two versions in mathematics of the abstract **dual lattice** concept, for a given lattice *L* in a real vector space *V*, of finite dimension.

The first, which generalises directly the reciprocal lattice construction, uses Fourier analysis. It may be stated simply in terms of Pontryagin duality. The dual group *V*^ to *V* is again a real vector space, and its closed subgroup *L*^ dual to *L* turns out to be a lattice in *V*^. Therefore, *L*^ is the natural candidate for *dual lattice*, in a different vector space (of the same dimension).

The other aspect is seen in the presence of a quadratic form $Q$ on $V$; if it is non-degenerate it allows an identification of the dual space $V^*$ of $V$ with $V$. The relation of $V^*$ to $V$ is not intrinsic; it depends on a choice of Haar measure (volume element) on $V$. But given an identification of the two, which is in any case well-defined up to a scalar, the presence of $Q$ allows one to speak to the dual lattice to $L$ while staying within $V$.

In mathematics, the **dual lattice** of a given lattice $L$ in an abelian locally compact topological group $G$ is the subgroup $L^*$ of the dual group of $G$ consisting of all continuous characters that are equal to one at each point of $L$.

In discrete mathematics, a lattice is a locally discrete set of points described by all integral linear combinations of dim = n linearly independent vectors in $R^n$. The dual lattice is then defined by all points in the linear span of the original lattice (typically all of R^n) with the property that an integer results from the inner product with all elements of the original lattice. It follows that the dual of the dual lattice is the original lattice.

Furthermore, if we allow the matrix B to have columns as the linearly independent vectors that describe the lattice, then the matrix

$A = B\left(B^{\mathsf{T}}B\right)^{-1}$ has columns of vectors that describe the dual lattice.

# Reciprocal space

Reciprocal space (also called "k-space") is the space in which the Fourier transform of a spatial function is represented (similarly the frequency domain is the space in which the Fourier transform of a time dependent function is represented). A Fourier transform takes us from "real space" to reciprocal space or *vice versa*. Reciprocal space comes into play regarding wave-mechanics: As a plane wave can be written by an oscillatory term $e^{i(kx-\omega t)}$ with wave vector $k$ and angular frequency $\omega$, it can be regarded as both a function of $k$ and $x$ (and the spectroscopic part as a function of both $\omega$ and $t$). In space, the periodicity oscillates with $kx = 2\pi$ - therefore for a given phase, $k$ and $x$ are reciprocal to each other: $k = 2\pi/x$ and $x = 2\pi/k$.

A reciprocal lattice is a periodic set of points in this space, and contains the $\vec{k}$ points that compose the Fourier transform of a periodic spatial lattice. The Brillouin zone is a volume within this space that contains all the unique k-vectors that represent the periodicity of classical or quantum waves allowed in a periodic structure.

# See also

- Crystallography
- Dual basis
- Ewald's sphere
- Miller index
- Powder diffraction
- Kikuchi line
- Brillouin zone
- Zone axis

# References


1. B. E. Warren (1969/1990) *X-ray diffraction* (Addison-Wesley, Reading MA/Dover, Mineola NY).


# External links

- http://newton.umsl.edu/run//nano/known.html - Jmol-based electron diffraction simulator lets you explore the intersection between reciprocal lattice and Ewald sphere during tilt.
- DoITPoMS Teaching and Learning Package on Reciprocal Space and the Reciprocal Lattice