

[reciprocal lattice]
 (Chapter 5.3 in *Elements*)

Reciprocal Lattice and Reciprocal Lattice Vectors

Reciprocal lattice vectors are 3-D vectors $\vec{\mathbf{k}}_i$ such that

$$\exp(i\vec{\mathbf{k}} \cdot \vec{\mathbf{r}}) = 1, \quad (5\text{-RL1})$$

where $\vec{\mathbf{r}}$ is the location of any (i.e., all) of the direct crystal lattice points,

$$\vec{\mathbf{r}}_{lmn} = \ell \vec{\mathbf{b}}_1 + m \vec{\mathbf{b}}_2 + n \vec{\mathbf{b}}_3 \quad (5\text{-RL2})$$

where ℓ, m, n are integers and $\vec{\mathbf{b}}_i$ are the (non coplanar) direct lattice basis vectors. Integer

combinations $\vec{\mathbf{Q}}_{pqr}$ of vectors $\vec{\mathbf{a}}_i = 2\pi \frac{\vec{\mathbf{b}}_j \otimes \vec{\mathbf{b}}_k}{V}$ (i, j, k in cyclic order), where $V = \vec{\mathbf{b}}_i \cdot \vec{\mathbf{b}}_j \otimes \vec{\mathbf{b}}_k$ is the volume of the direct lattice cell, satisfy the condition (RL1). The set of all such vectors $\vec{\mathbf{Q}}_{pqr} = p\vec{\mathbf{k}}_i + q\vec{\mathbf{k}}_j + r\vec{\mathbf{k}}_k$ (integers p, q, r) then form a lattice, which is in one-to-one relation to the direct lattice, because

$$\vec{\mathbf{b}}_i = \frac{1}{2\pi} \vec{\mathbf{k}}_j \otimes \vec{\mathbf{k}}_k. \quad (5\text{-RL3})$$

The $\vec{\mathbf{Q}}_{pqr}$ -lattice is called the *reciprocal lattice* and the $\vec{\mathbf{a}}_i$ s are the *basis* of the reciprocal lattice.