Reciprocal Lattice

Plane wave : $\psi_k(r) = \psi_0 e^{i\vec{k}.\vec{r}}$

Real space Bravais Lattice [Direct Lattice] : $\vec{R} = m\vec{a_1} + n\vec{a_2} + o\vec{a_3}$

$m, n, o \in Z$ and $\vec{a_1}, \vec{a_2}, \vec{a_3}$ are primitive vectors.

Reciprocal lattice : Set of wave vectors $\vec{k}$ for which

$$\psi_k(\vec{r}) = \psi_k(\vec{r}+\vec{R})$$

$$\psi_0 . e^{i\vec{k}.\vec{r}} = \psi_0 . e^{i\vec{k}.(\vec{r}+\vec{R})}$$

$$e^{i\vec{k}.\vec{R}} = 1$$

$$\Rightarrow \vec{k}.\vec{R} = 2\pi l, \; l \in Z. \longrightarrow (1)$$

<u>Lattice vectors for Reciprocal Lattice</u> : $\vec{k} = p\vec{b_1} + q\vec{b_2} + r\vec{b_3}$, p, q, r are coefficients.

Eqn. (1) gives

$$(p\ q\ r)\begin{pmatrix} \vec{b_1}.\vec{a_1} & \vec{b_1}.\vec{a_2} & b_1.\vec{a_3} \\ \vec{b_2}.\vec{a_1} & \cdots & \\ \vec{b_3}.\vec{a_1} & \vdots & \vec{b_3}.\vec{a_3} \end{pmatrix}\begin{pmatrix} m \\ n \\ o \end{pmatrix} = 2\pi l \quad -(2)$$

Choose the simplest basis $\{\vec{b_i}\}$ for vectors $\vec{k}$,

$$\vec{b_i}.\vec{a_j} = 2\pi \delta_{ij} \quad -(3)$$

Combining (2) & (3), and dividing by 2π,

$$pm + qn + ro = l$$

Since m, n, o are arbitrary integers and l is also an integer, <u>p, q, r must also be integers</u>.

$\therefore$ <u>$\vec{k} = p\vec{b_1} + q\vec{b_2} + r\vec{b_3}$</u> also forms a Bravais lattice.