An historical introduction to the reciprocal lattice

Didactic material for the MaThCryst schools

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Morphology and stereographic projection (reminder)
Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

Auguste Bravais (1811-1863)
Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

\[ \mathbf{a} \times \mathbf{b} = S(001) \]

\[ \mathbf{e}_{(001)} = \frac{\mathbf{a} \times \mathbf{b}}{||\mathbf{a} \times \mathbf{b}||} \]

\[ V = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}) = S(001)d_{(001)} = S(hkl)d_{(hkl)} \]
Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

The vector space $V^n$ is realized with a metric in Å obeying the above conditions.
Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

By construction, the vector $[hkl]^p$ is perpendicular to the face $(hkl)$
Angles between vectors of the polar lattice are precisely the angles between face normals.

\[
\delta = \pi - \varphi
\]

\[
\cos \delta = \frac{\mathbf{r}_1^p \cdot \mathbf{r}_2^p}{\|\mathbf{r}_1^p\| \cdot \|\mathbf{r}_2^p\|} = \frac{\begin{vmatrix} h_1 & k_1 & l_1 \end{vmatrix}G^p}{\begin{vmatrix} h_1 & k_1 & l_1 \end{vmatrix}}\frac{\begin{vmatrix} h_2 \\ k_2 \\ l_2 \end{vmatrix}}{\begin{vmatrix} h_2 \\ k_2 \\ l_2 \end{vmatrix}}
\]

\[
G^p = \begin{pmatrix} a^p \cdot a^p & a^p \cdot b^p & a^p \cdot c^p \\ b^p \cdot a^p & b^p \cdot b^p & b^p \cdot c^p \\ c^p \cdot a^p & c^p \cdot b^p & c^p \cdot c^p \end{pmatrix}
\]
Use of the polar lattice makes indexing of stereographic poles straightforward – monoclinic example

Parallel to $a$ and $b$ axes
On the $c^p$ axis

Parallel to $c$ and $b$ axes
On the $a^p$ axis

Parallel to $a$ and $b$ axes
On the $c^p$ axis

(001)
(100)
Use of the polar lattice makes indexing of stereographic poles straightforward – hexagonal example

- Parallel to $A_2$ and $C$ axes
- On the $a^p$ axis
- Same intersection on $A_1$ and $A_2$ (positive)
- Half intersection on $A_3$ (negative)
- On the bisector of $a^p$ and $b^p$
Use of the polar lattice makes indexing of stereographic poles straightforward – hexagonal example
Then, something happened....

Wilhelm Conrad Röntgen
(1845-1923)
1895 : discovery of X-rays
1912: crystals diffract X-rays

Max von Laue
(1879-1960)
1912: crystals diffract X-rays

X-ray diffraction pattern of ZnS by Friedrich, Knipping and Laue
A diffraction pattern can be indexed with a lattice whose metric is inverse (reciprocal) of the Bravais lattices.

Diffractions make a lattice that can be indexed on the basis of suitably chosen axes.
1913: the reciprocal lattice

Paul Peter Ewald (1888-1985)
The reciprocal lattice

$a^* = (b \times c)/V$, $b^* = (c \times a)/V$, $c^* = (a \times b)/V \quad \text{Å}^{-1}$ !

The reciprocal lattice

The reciprocal space is a vector space $V^n$ realized with a metric in $\text{Å}^{-1}$
Linear parameters of the reciprocal lattice

\[ a^* = (b \times c)/V, \quad b^* = (c \times a)/V, \quad c^* = (a \times b)/V \]

\[ a^* = bcsin\alpha/V, \quad b^* = casin\beta/V, \quad c^* = absin\gamma/V \]

\[ a \cdot a^* = a \cdot (b \times c)/V = 1 ; \quad b \cdot b^* = b \cdot (c \times a)/V = 1 ; \quad c \cdot c^* = c \cdot (a \times b)/V = 1 \]

\[ \nu_i \cdot \nu_j^* = \delta_{ij} \]

\[ V^* = a^* \cdot b^* \times c^* = (b \times c) \cdot (c \times a) \times (a \times b)/V^3 = (b \times c) \cdot [(c \cdot a \times b)a-(c \cdot a \times a)b]/V^3 = (b \times c) \cdot [Va-0b]/V^3 = V^2/V^3 = 1/V \]

\[ a = (b^* \times c^*)/V^* ; \quad b = (c^* \times a^*)/V^* ; \quad c = (a^* \times b^*)/V^* \]
Angular parameters of the reciprocal lattice

\[ a^* = bcsin\alpha/V, \quad b^* = casin\beta/V, \quad c^* = absin\gamma/V \]

\[ a = b^*c^*sin\alpha*/V* \quad ; \quad b^* = a^*c^*sin\beta*/V* \quad ; \quad c^* = a^*b^*sin\gamma*/V* \quad (V^* = 1/V) \]

\[ \sin \alpha^* = \frac{a V^*}{b^* c^*} = \frac{a}{V} \frac{V}{abc \sin \beta \sin \gamma} \]

\[ \sin \beta^* = \frac{b V^*}{a^* c^*} = \frac{b}{V} \frac{V}{abc \sin \alpha \sin \gamma} \]

\[ \sin \gamma^* = \frac{c V^*}{a^* b^*} = \frac{c}{V} \frac{V}{abc \sin \alpha \sin \beta} \]
Metric tensor of the reciprocal lattice

\[ G^* = \begin{pmatrix} a^* \cdot a^* & a^* \cdot b^* & a^* \cdot c^* \\ b^* \cdot a^* & b^* \cdot b^* & b^* \cdot c^* \\ c^* \cdot a^* & c^* \cdot b^* & c^* \cdot c^* \end{pmatrix} \]

\[ G^* = G^{-1} \ ; \ det(G^*) = 1/det(G) \Rightarrow V^* = 1/V \]

Angles between the \( (h_1k_1l_1) \) and \( (h_2k_2l_2) \) faces computed as angle between \( r^*(h_1k_1l_1) \) and \( r^*(h_2k_2l_2) \) vectors

\[ \cos \left( h_1 \ k_1 \ l_1 \right)^\wedge \left( h_2 \ k_2 \ l_2 \right) = \frac{\langle h_1 \ k_1 \ l_1 | G^* | h_2 \ k_2 \ l_2 \rangle}{\sqrt{\langle h_1 \ k_1 \ l_1 | G^* | h_1 \ k_1 \ l_1 \rangle} \sqrt{\langle h_2 \ k_2 \ l_2 | G^* | h_2 \ k_2 \ l_2 \rangle}} \]
Equidistance of lattice planes

\[ e_{hkl}^* = r_{hkl}^* / \| r_{hkl}^* \| \]

\[ d_{(hkl)} = e_{hkl}^* \cdot a/h \]

\[ d_{(hkl)} = e_{hkl}^* \cdot b/k \]

\[ d_{(hkl)} = e_{hkl}^* \cdot c/l \]

\[
\begin{align*}
    d(hkl) &= \frac{a \cdot h a^* + k b^* + l c^*}{\| r_{hkl}^* \|} = \frac{h1 + h0 + l0}{h \| r_{hkl}^* \|} = \frac{1}{r_{hkl}^*} \\
    d(hkl) &= \frac{b \cdot h a^* + k b^* + l c^*}{\| r_{hkl}^* \|} = \frac{h0 + h1 + l0}{k \| r_{hkl}^* \|} = \frac{1}{r_{hkl}^*} \\
    d(hkl) &= \frac{c \cdot h a^* + k b^* + l c^*}{\| r_{hkl}^* \|} = \frac{h0 + h0 + l1}{l \| r_{hkl}^* \|} = \frac{1}{r_{hkl}^*}
\end{align*}
\]
Not really Ewald's discovery....

Reciprocal system of vectors (1881)

Josiah Willard Gibbs
(1839-1903)
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