An historical introduction to the reciprocal lattice

Didactic material for the MaThCryst schools

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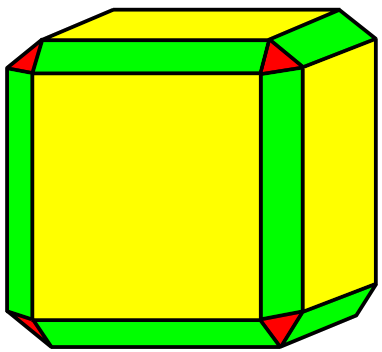
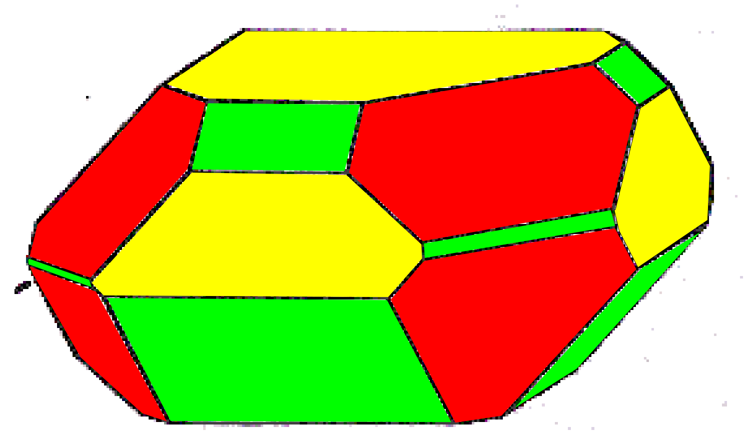
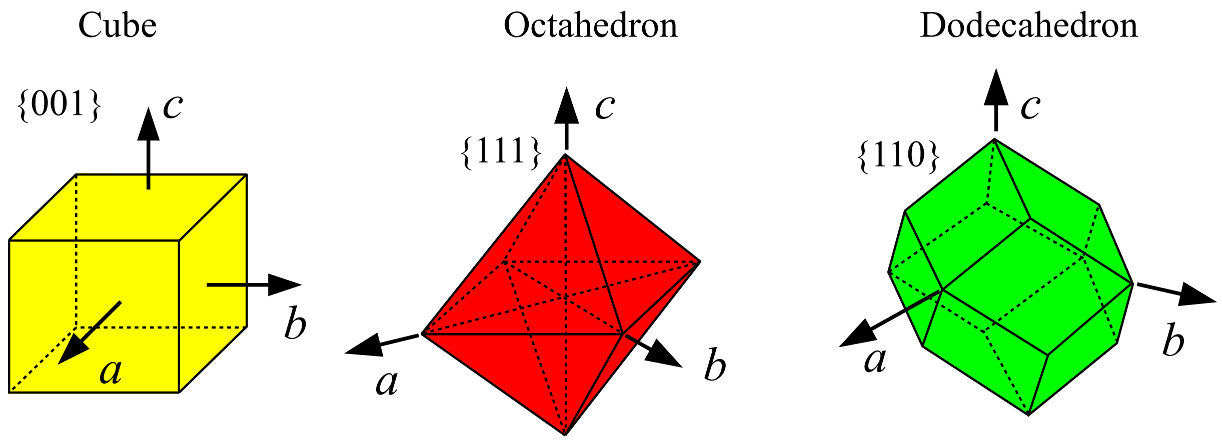
Morphology and stereographic projection (reminder)



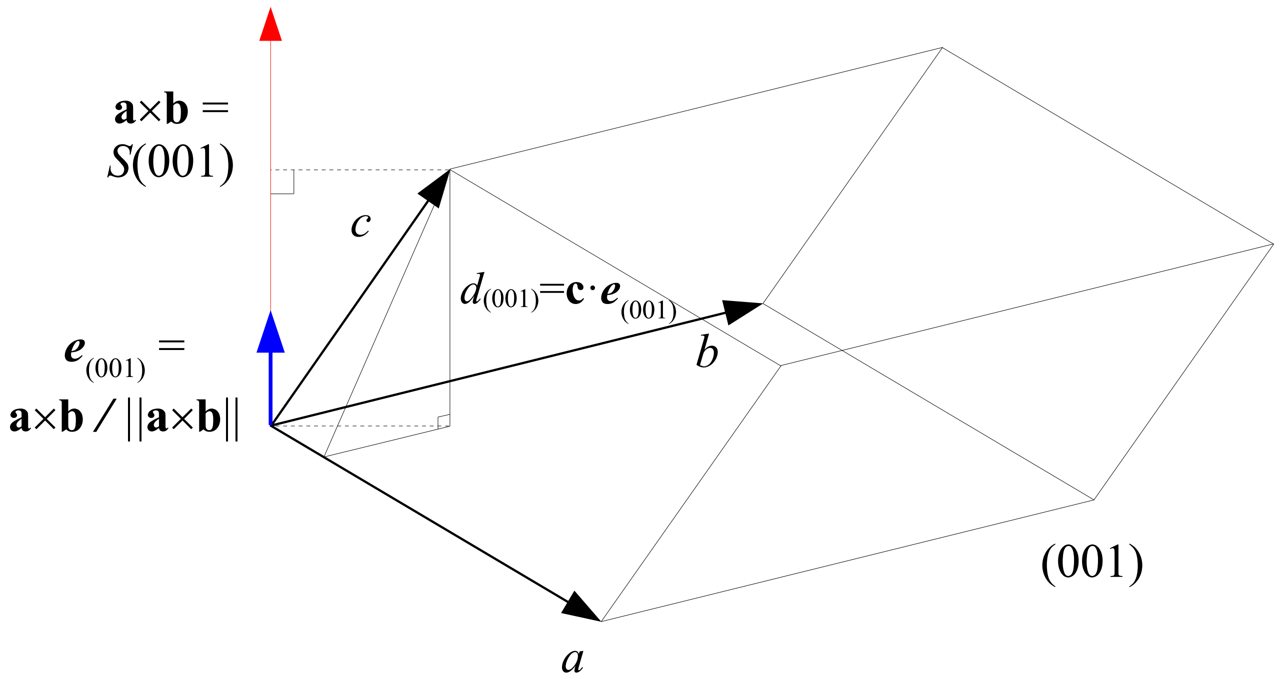




Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

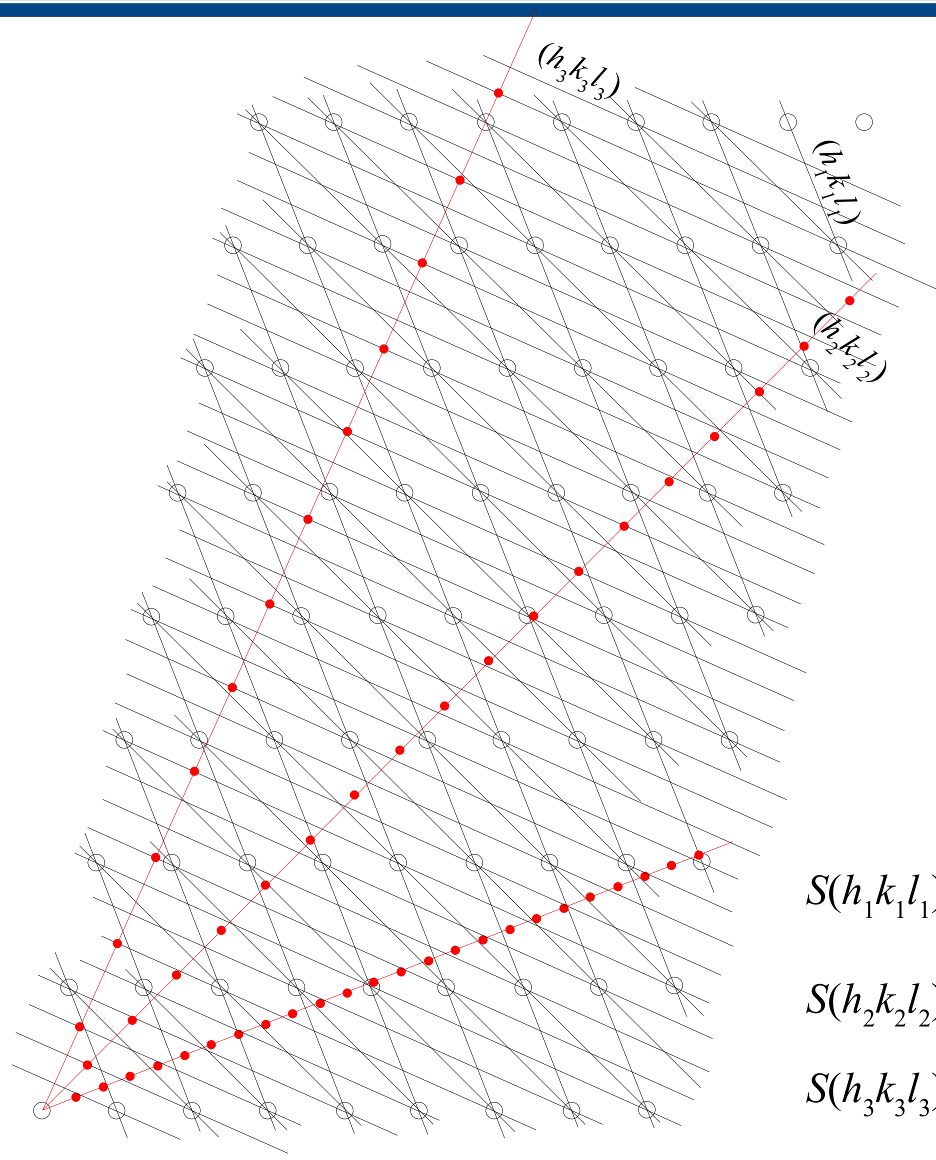
Auguste Bravais (1811-1863)

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



$$V = \mathbf{c}\cdot\mathbf{a}\times\mathbf{b} = S(001)d_{(001)} = S(hkl)d_{(hkl)}$$

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



Polar lattice (in vector space)

$S(h_1k_1l_1)/V^{1/3}$ (Å)

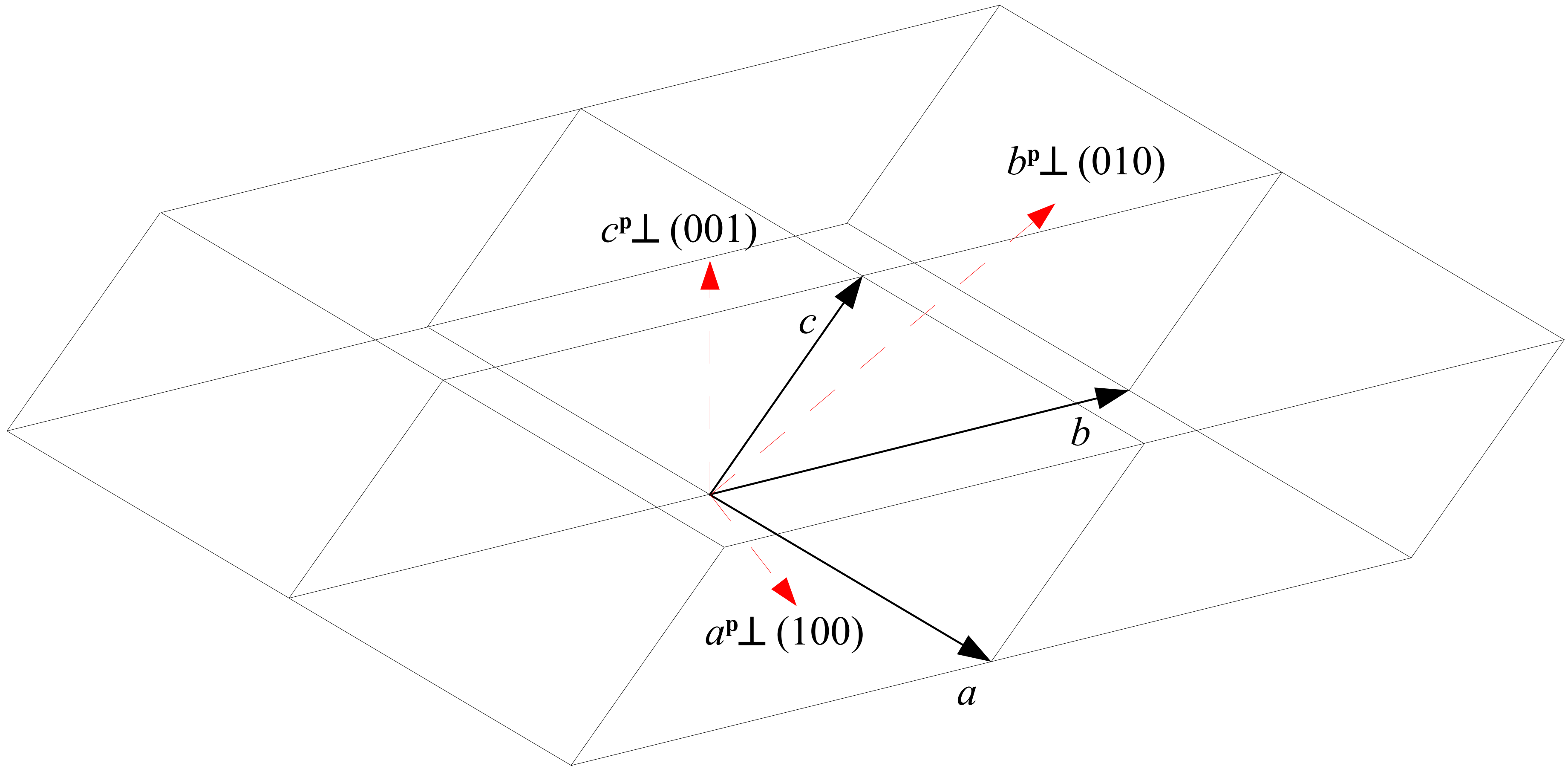
$S(h_2k_2l_2)/V^{1/3}$ (Å)

$S(h_3k_3l_3)/V^{1/3}$ (Å)

$$\|\mathbf{r}^{p}_{hkl}\| = S(hkl)/V^{1/3} = [V/d_{(hkl)}]/V^{1/3} = V^{2/3}/d_{(hkl)} \quad (\text{Å})$$

The vector space $\mathbf{V}^n$ 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

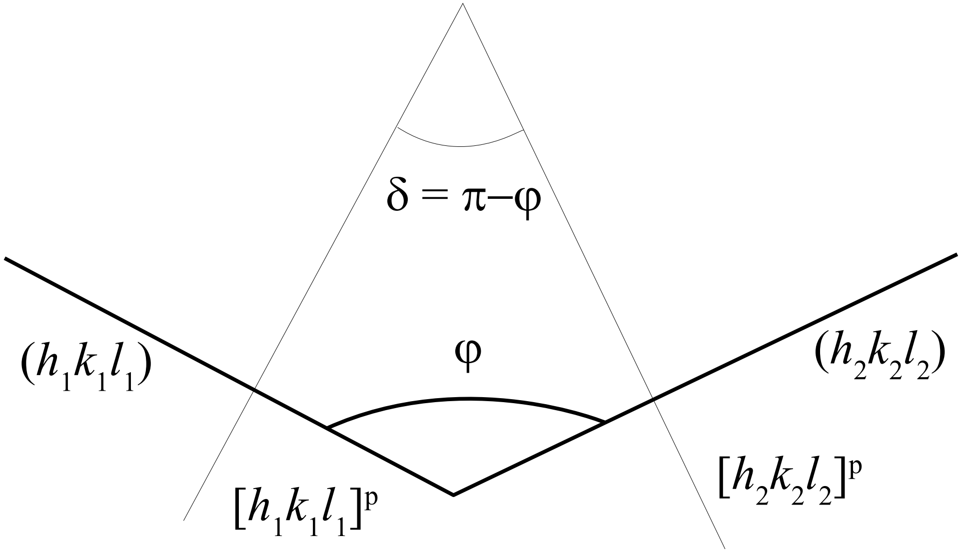


$$\boldsymbol{a}^{\mathrm{p}}=\frac{S(100)}{\mathrm{V}^{1/3}}=\frac{\boldsymbol{b}\times\boldsymbol{c}}{\mathrm{V}^{1/3}};\quad \boldsymbol{b}^{\mathrm{p}}=\frac{S(010)}{\mathrm{V}^{1/3}}=\frac{\boldsymbol{c}\times\boldsymbol{a}}{\mathrm{V}^{1/3}};\quad \boldsymbol{a}^{\mathrm{p}}=\frac{S(001)}{\mathrm{V}^{1/3}}=\frac{\boldsymbol{a}\times\boldsymbol{b}}{\mathrm{V}^{1/3}}$$

$$\boldsymbol{v}_{\mathrm{i}}\cdot\boldsymbol{v}_{\mathrm{j}}^{\mathrm{p}}=m\delta_{\mathrm{ij}}\qquad m=\boldsymbol{v}_i\cdot\boldsymbol{v}_i^p=\boldsymbol{v}_i\cdot\frac{\boldsymbol{v}_j\times\boldsymbol{v}_k}{\mathrm{V}^{1/3}}=\frac{\mathrm{V}}{\mathrm{V}^{1/3}}=\mathrm{V}^{2/3}$$

By construction, the vector $[hkl]^{\mathrm{p}}$ is perpendicular to the face (hkl)

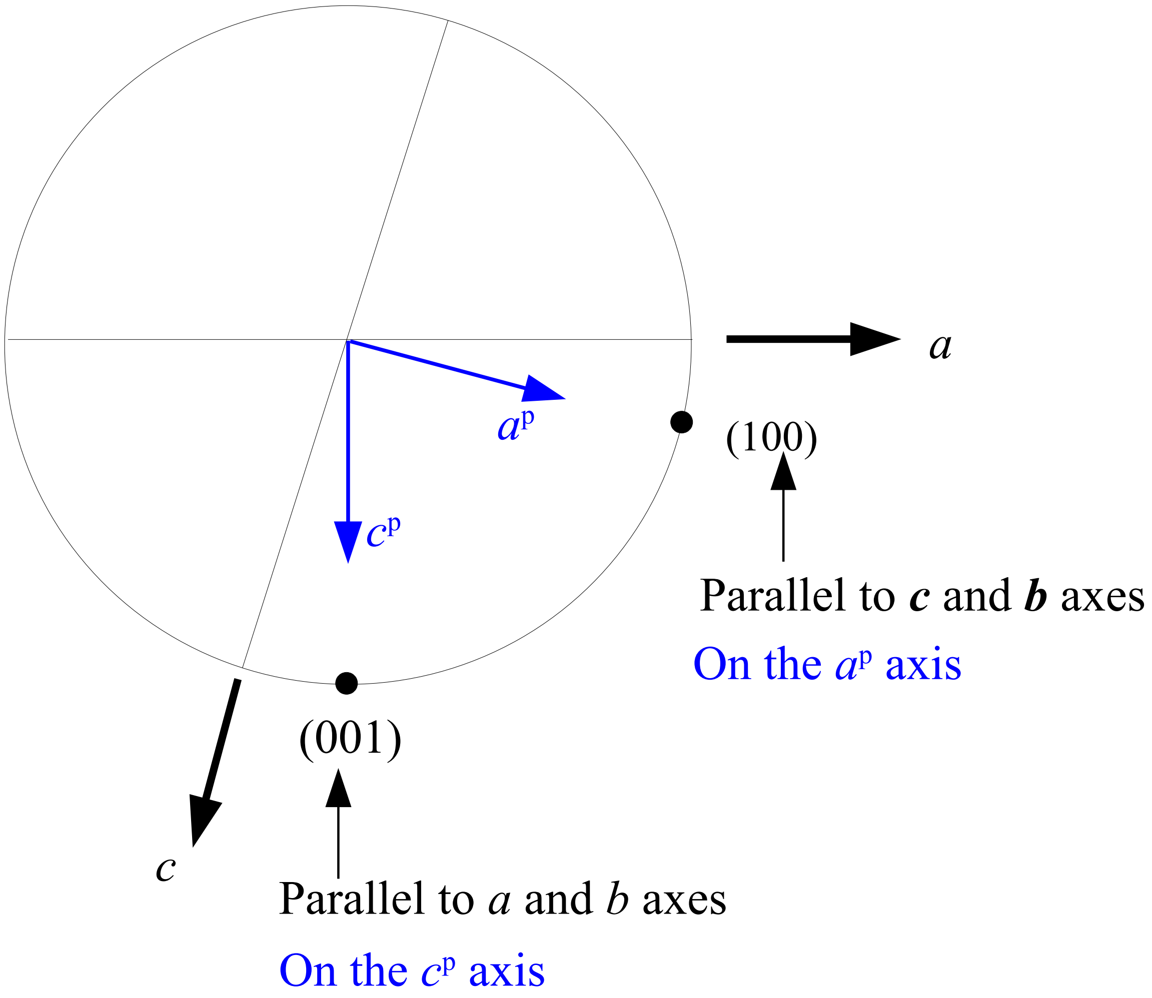
Angles between vectors of the polar lattice are precisely the angles between face normals



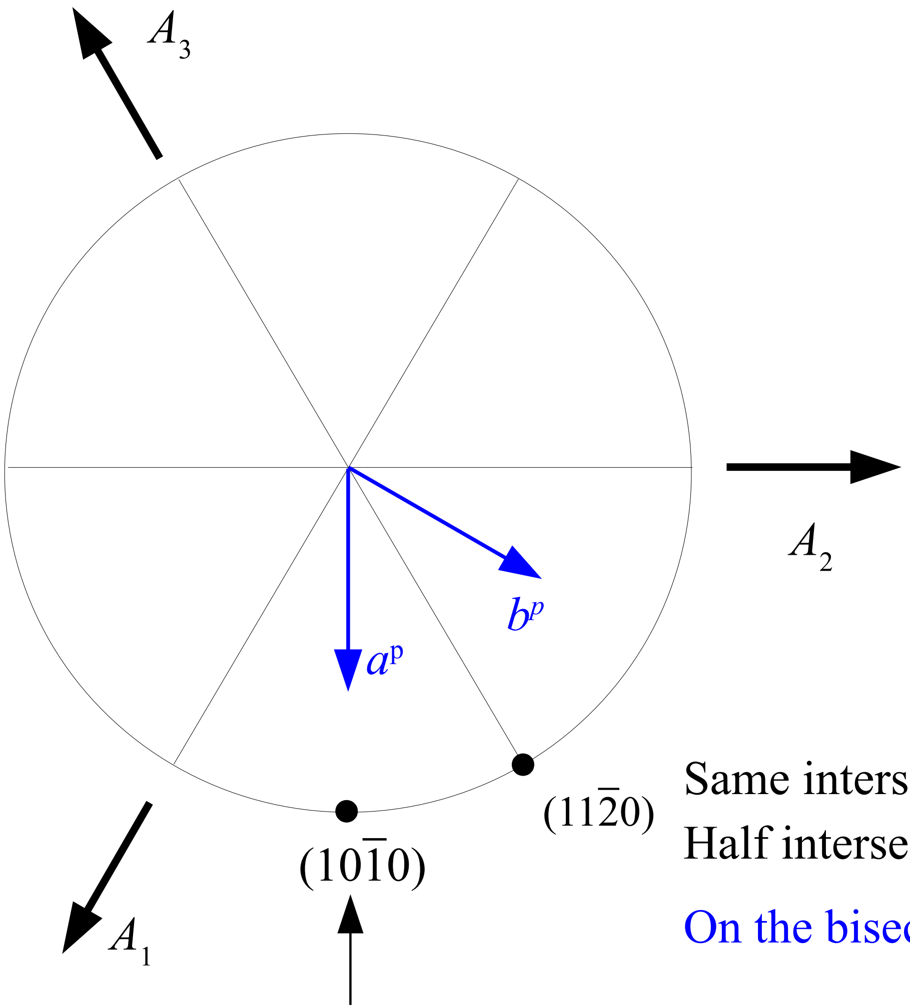
$$\cos\delta = \mathbf{r}_1{}^{p}\cdot\mathbf{r}_2{}^{p} / \|\mathbf{r}_1{}^{p}\|\cdot\|\mathbf{r}_2{}^{p}\| = \frac{\begin{pmatrix} h_1 & k_1 & l_1 \end{pmatrix} \mathbf{G}^{p} \begin{pmatrix} h_2 \\ k_2 \\ l_2 \end{pmatrix}}{\sqrt{\begin{pmatrix} h_1 & k_1 & l_1 \end{pmatrix} \mathbf{G}^{p} \begin{pmatrix} h_1 \\ k_1 \\ l_1 \end{pmatrix}}\sqrt{\begin{pmatrix} h_2 & k_2 & l_2 \end{pmatrix} \mathbf{G}^{p} \begin{pmatrix} h_2 \\ k_2 \\ l_2 \end{pmatrix}}}$$

$$\mathbf{G}^{p} = \begin{pmatrix} \mathbf{a}^{p}\cdot\mathbf{a}^{p} & \mathbf{a}^{p}\cdot\mathbf{b}^{p} & \mathbf{a}^{p}\cdot\mathbf{c}^{p} \\ \mathbf{b}^{p}\cdot\mathbf{a}^{p} & \mathbf{b}^{p}\cdot\mathbf{b}^{p} & \mathbf{b}^{p}\cdot\mathbf{c}^{p} \\ \mathbf{c}^{p}\cdot\mathbf{a}^{p} & \mathbf{c}^{p}\cdot\mathbf{b}^{p} & \mathbf{c}^{p}\cdot\mathbf{c}^{p} \end{pmatrix}$$

Use of the polar lattice makes indexing of stereographic poles straightforward – monoclinic example



Use of the polar lattice makes indexing of stereographic poles straightforward – hexagonal example



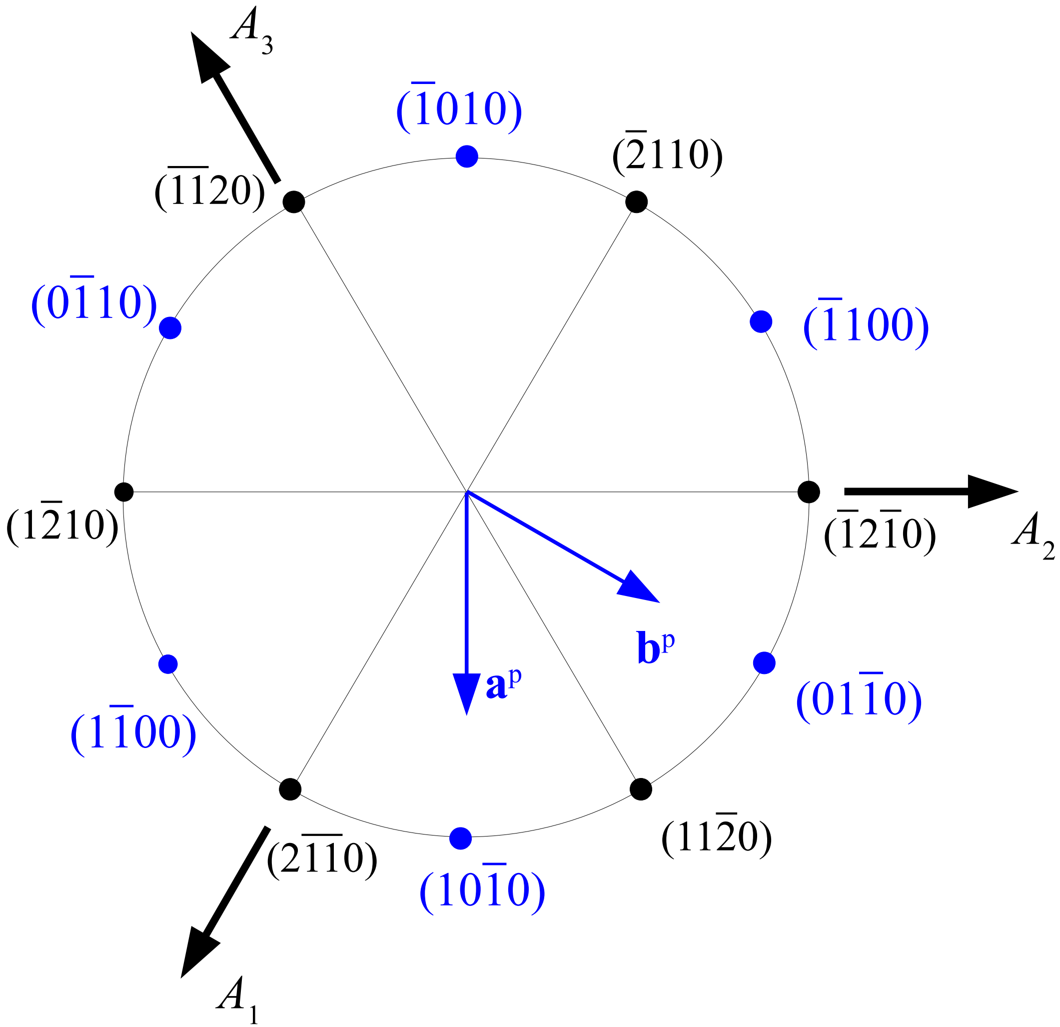
Same intersection on A_1 and A_2 (positive)
Half intersection on A_3 (negative)

On the bisector of a^p and b^p

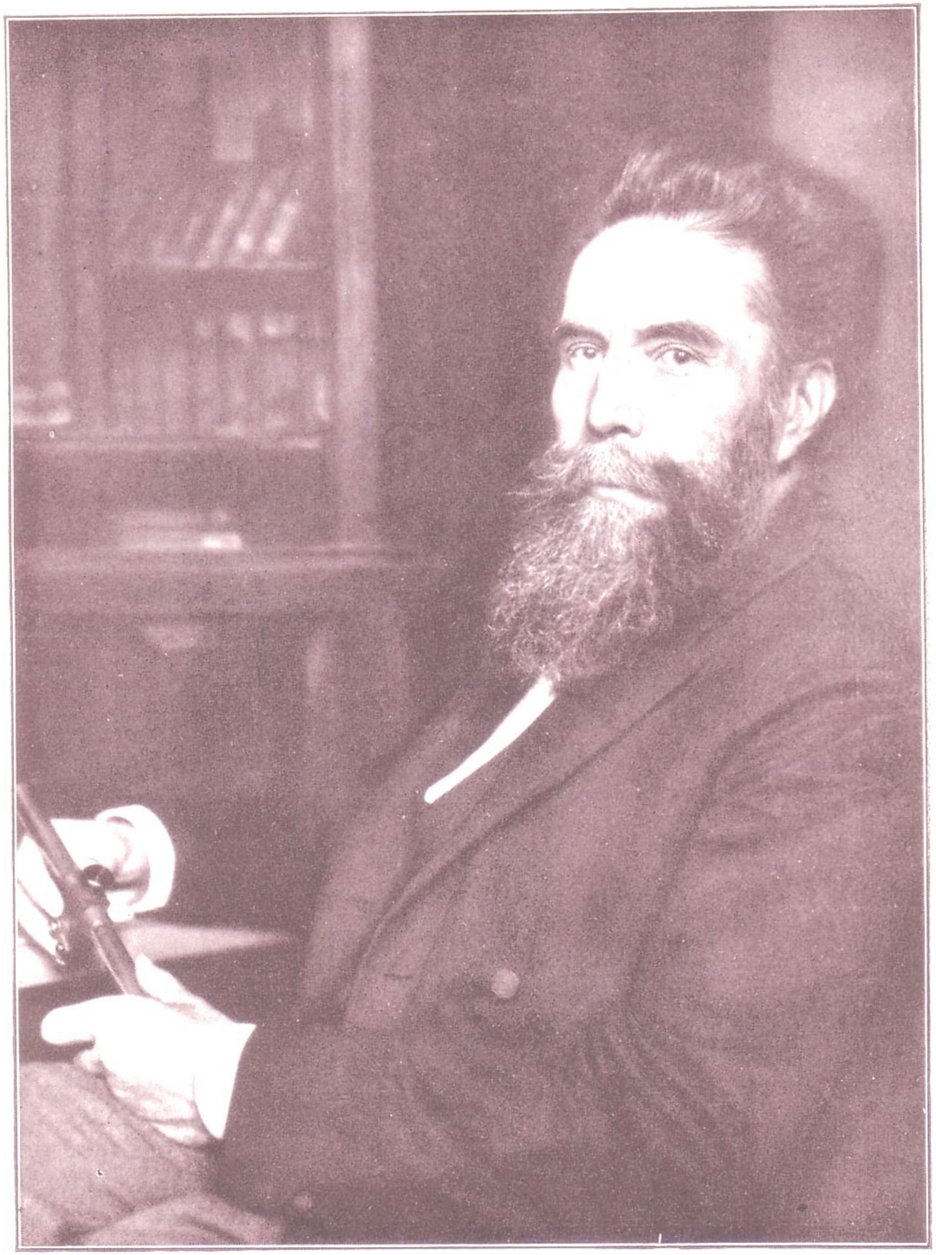
Parallel to A_2 and C axes

On the a^p axis

Use of the polar lattice makes indexing of stereographic poles straightforward – hexagonal example

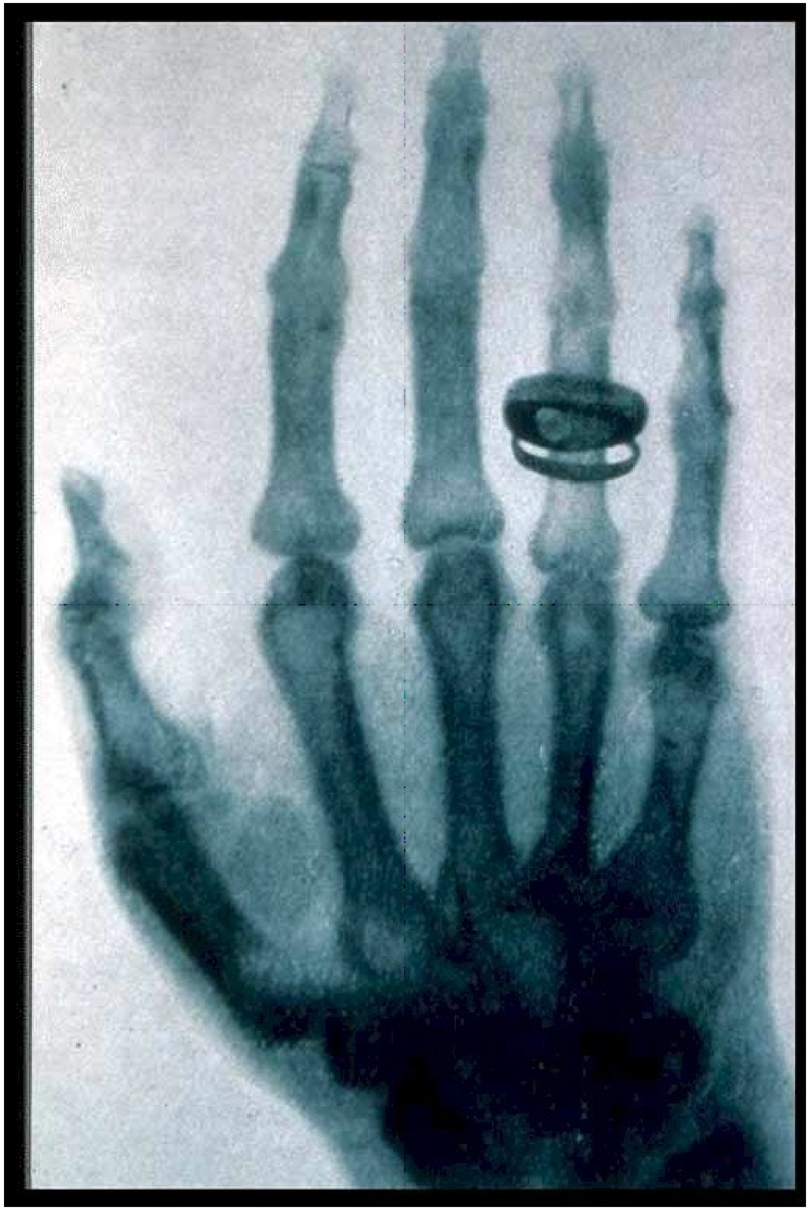


Then, something happened....



Wilhelm Conrad Röntgen
(1845-1923)

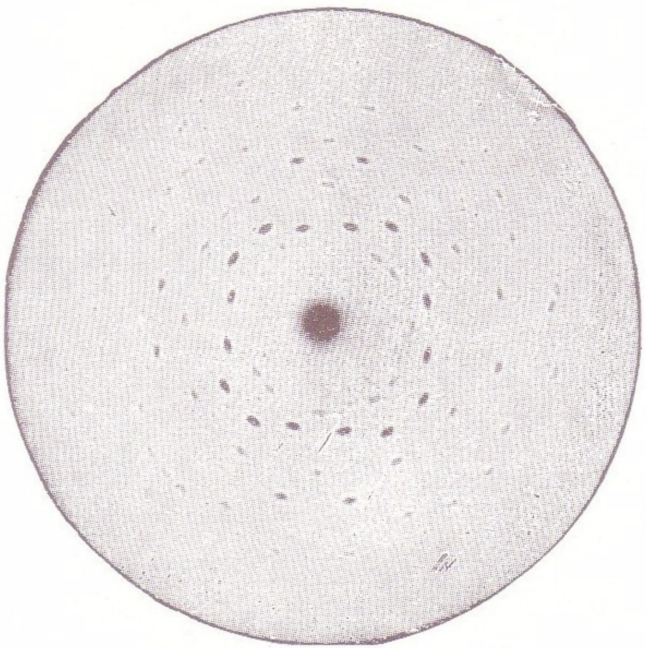
1895 : discovery of X-rays



1912: crystals diffract X-rays

Max von Laue
(1879-1960)

1912: crystals diffract X-rays



Laue effect for a zinc-blende plate parallel to a cubic surface

Laue effect for a zinc-blende plate parallel to a tetrahedral surface

X-ray diffraction pattern of ZnS by Friedrich, Knipping and Laue

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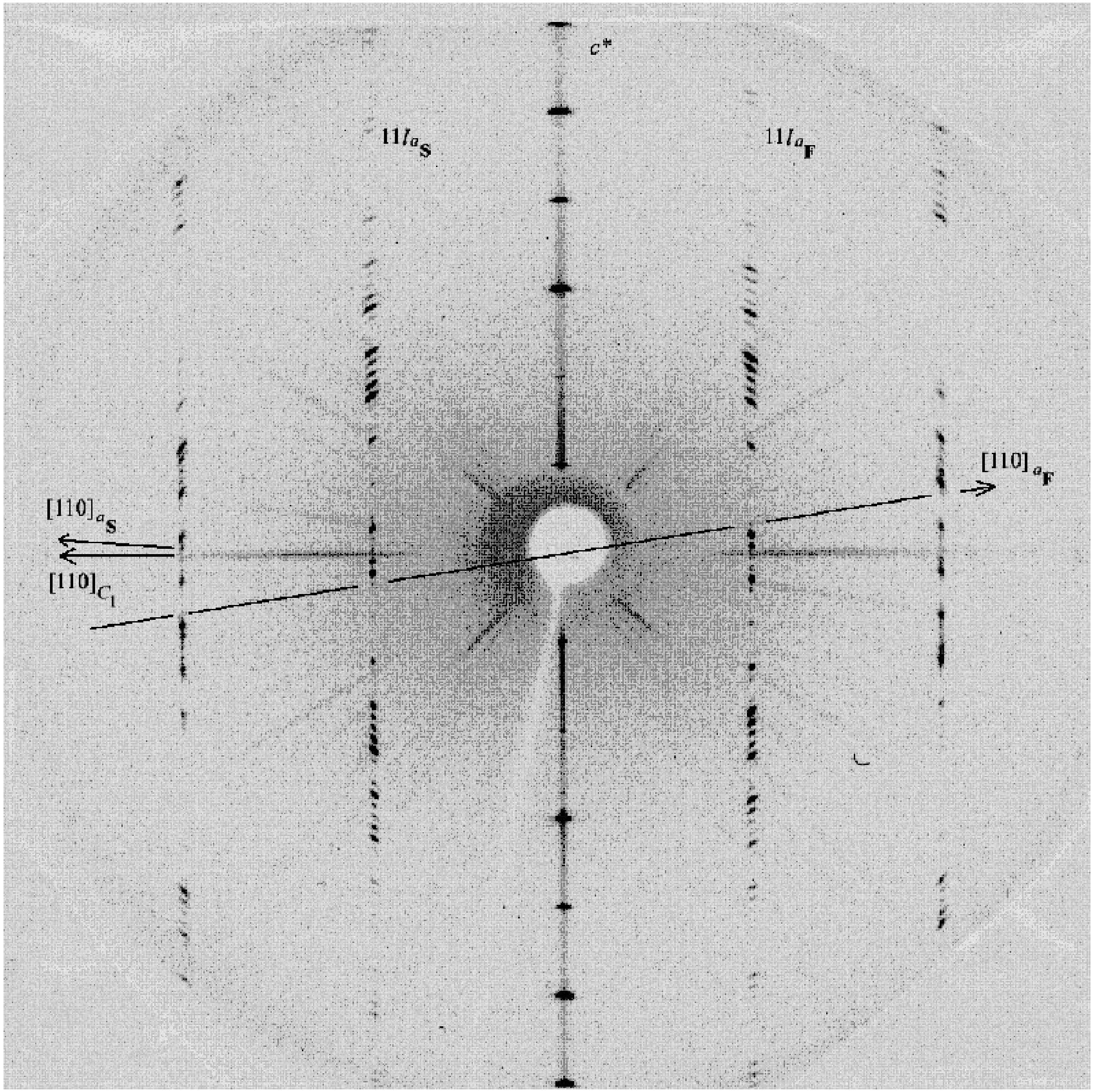
A diffraction pattern can be indexed with a lattice whose metric is inverse (reciprocal) of the Bravais lattices



Diffractions make a lattice that can be indexed on the basis of suitably chosen axes

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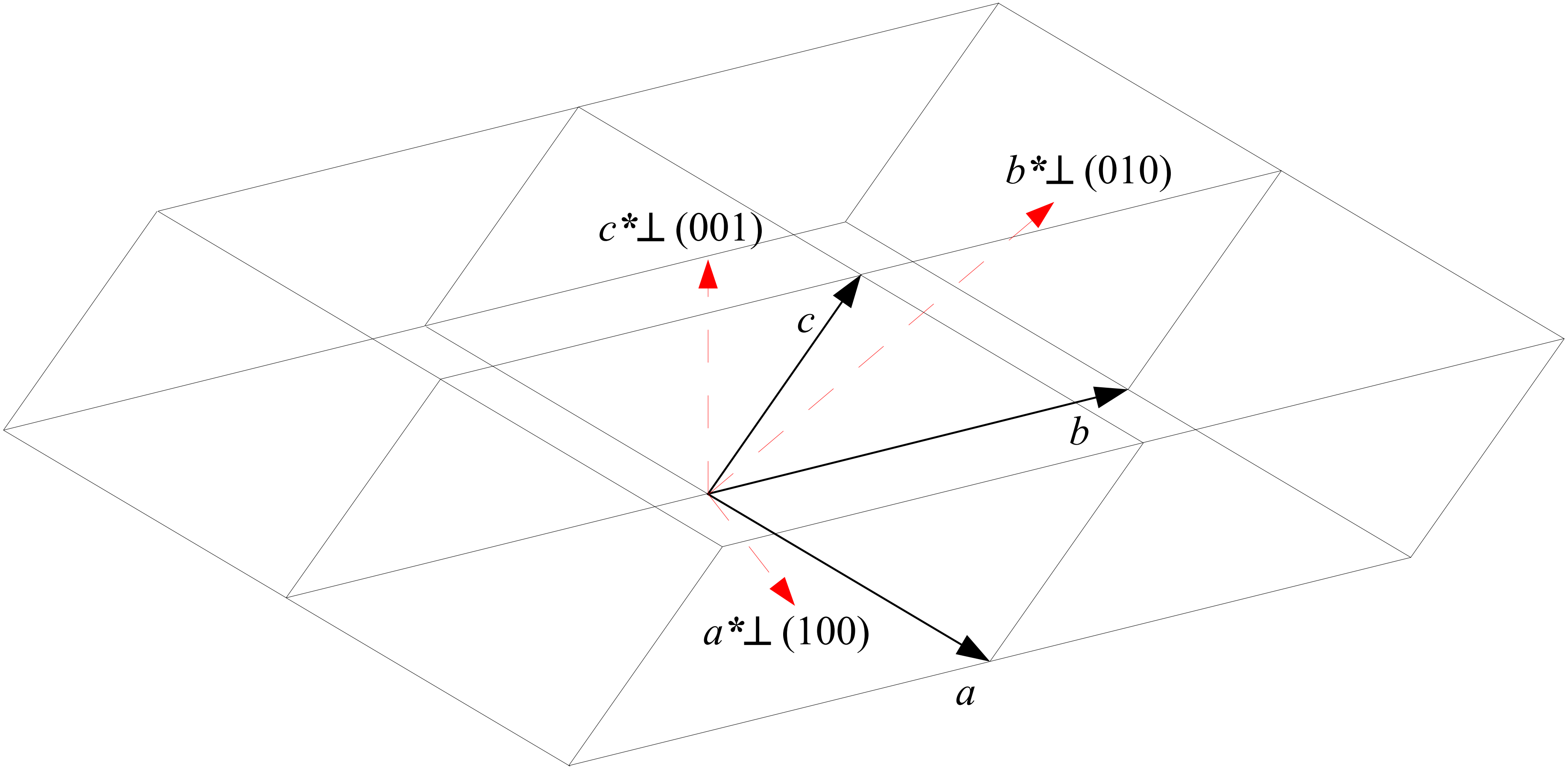
1913 : the reciprocal lattice

Paul Peter Ewald (1888-1985)

1913 : the reciprocal lattice



a* = (b×c)/V, b* = (c×a)/V, c* = (a×b)/V **Å^{-1} !**

The reciprocal lattice

The reciprocal space is a vector space **V**^{n} realized with a metric in Å^{-1}

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Linear parameters of the reciprocal lattice

$$\mathbf{a}^* = (\mathbf{b}\times\mathbf{c})/V,\ \mathbf{b}^* = (\mathbf{c}\times\mathbf{a})/V,\ \mathbf{c}^* = (\mathbf{a}\times\mathbf{b})/V$$

$$a^* = bc\sin\alpha/V,\ b^* = ca\sin\beta/V,\ c^* = ab\sin\gamma/V$$

$$\mathbf{a}\cdot\mathbf{a}^* = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})/V = 1\ ;\ \mathbf{b}\cdot\mathbf{b}^* = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a})/V = 1\ ;\ \mathbf{c}\cdot\mathbf{c}^* = \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b})/V = 1$$

$$\boldsymbol{v}_i\cdot\boldsymbol{v}_j^* = \delta_{ij}$$

$$V^* = \mathbf{a}^*\cdot\mathbf{b}^*\times\mathbf{c}^* = (\mathbf{b}\times\mathbf{c})\cdot(\mathbf{c}\times\mathbf{a})\times(\mathbf{a}\times\mathbf{b})/V^3 = (\mathbf{b}\times\mathbf{c})\cdot[(\mathbf{c}\cdot\mathbf{a}\times\mathbf{b})\mathbf{a}-(\mathbf{c}\cdot\mathbf{a}\times\mathbf{a})\mathbf{b}]/V^3 =$$

$$(\mathbf{b}\times\mathbf{c})\cdot[V\mathbf{a}-0\mathbf{b}]/V^3 = V^2/V^3 = 1/V$$

$$\mathbf{a} = (\mathbf{b}^*\times\mathbf{c}^*)/V^*\ ;\ \mathbf{b} = (\mathbf{c}^*\times\mathbf{a}^*)/V^*\ ;\ \mathbf{c} = (\mathbf{a}^*\times\mathbf{b}^*)/V^*$$

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Angular parameters of the reciprocal lattice

$$a^* = bc\sin\alpha/V,\; b^* = ca\sin\beta/V,\; c^* = ab\sin\gamma/V$$

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

$$\sin\alpha^* = \frac{a\,V^*}{b^*c^*} = \frac{\frac{a}{V}}{\frac{ac\sin\beta}{V}\frac{ab\sin\gamma}{V}} = \frac{V}{abc\sin\beta\sin\gamma}$$

$$\sin\beta^* = \frac{b\,V^*}{a^*c^*} = \frac{\frac{b}{V}}{\frac{bc\sin\alpha}{V}\frac{ab\sin\gamma}{V}} = \frac{V}{abc\sin\alpha\sin\gamma}$$

$$\sin\gamma^* = \frac{c\,V^*}{a^*b^*} = \frac{\frac{c}{V}}{\frac{bc\sin\alpha}{V}\frac{ac\sin\beta}{V}} = \frac{V}{abc\sin\alpha\sin\beta}$$

Metric tensor of the reciprocal lattice

$$\mathbf{G}^* = \begin{pmatrix} \mathbf{a}^*\cdot\mathbf{a}^* & \mathbf{a}^*\cdot\mathbf{b}^* & \mathbf{a}^*\cdot\mathbf{c}^* \\ \mathbf{b}^*\cdot\mathbf{a}^* & \mathbf{b}^*\cdot\mathbf{b}^* & \mathbf{b}^*\cdot\mathbf{c}^* \\ \mathbf{c}^*\cdot\mathbf{a}^* & \mathbf{c}^*\cdot\mathbf{b}^* & \mathbf{c}^*\cdot\mathbf{c}^* \end{pmatrix}$$

$$\mathbf{G}^* = \mathbf{G}^{-1} \quad ; \det(\mathbf{G}^*) = 1/\det(\mathbf{G}) \Rightarrow V^* = 1/V$$

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

$$\cos\left(h_1\ k_1\ l_1\right)\wedge\left(h_2\ k_2\ l_2\right) = \frac{\left\langle h_1\ k_1\ l_1 \middle| \mathbf{G}^* \middle| h_2\ k_2\ l_2 \right\rangle}{\sqrt{\left\langle h_1\ k_1\ l_1 \middle| \mathbf{G}^* \middle| h_1\ k_1\ l_1 \right\rangle}\sqrt{\left\langle h_2\ k_2\ l_2 \middle| \mathbf{G}^* \middle| h_2\ k_2\ l_2 \right\rangle}}$$

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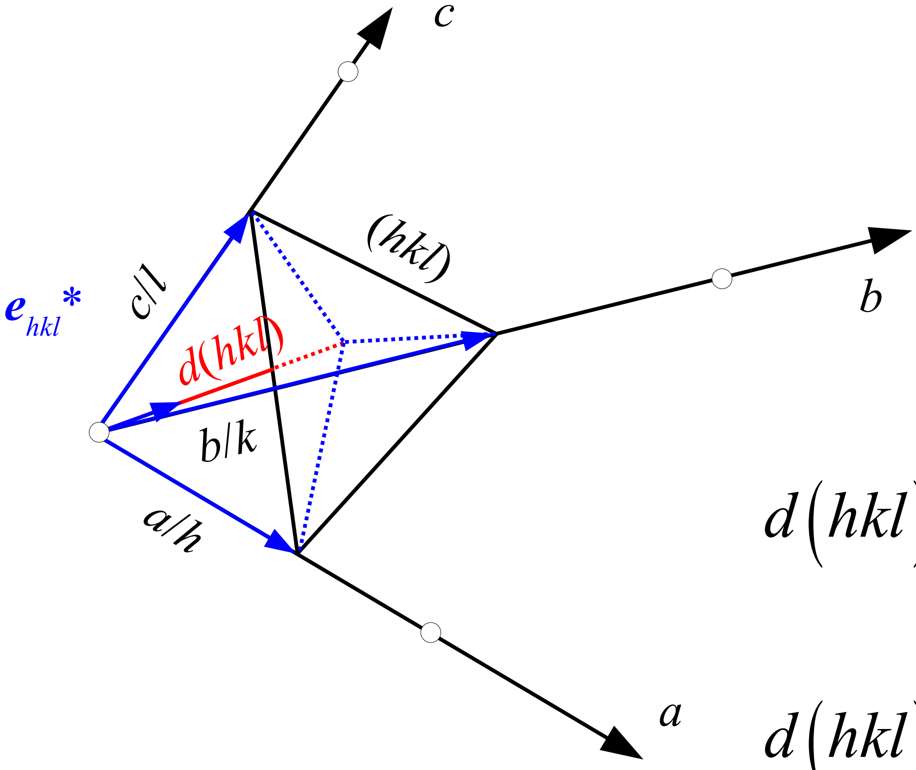
Equidistance of lattice planes



$$\boldsymbol{e}_{hkl}^* = \mathbf{r}_{hkl}^* / \|\mathbf{r}_{hkl}^*\|$$

$$\boldsymbol{d}_{(hkl)} = \boldsymbol{e}_{hkl}^* \cdot \mathbf{a}/h$$

$$\boldsymbol{d}_{(hkl)} = \boldsymbol{e}_{hkl}^* \cdot \mathbf{b}/k$$

$$\boldsymbol{d}_{(hkl)} = \boldsymbol{e}_{hkl}^* \cdot \mathbf{c}/l$$

$$d(hkl) = \frac{\mathbf{a}}{h} \cdot \frac{h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*}{\|\mathbf{r}_{hkl^*}\|} = \frac{h1 + h0 + l0}{h\|\mathbf{r}_{hkl^*}\|} == \frac{1}{\|\mathbf{r}_{hkl^*}\|}$$

$$d(hkl) = \frac{\mathbf{b}}{k} \cdot \frac{h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*}{\|\mathbf{r}_{hkl^*}\|} = \frac{h0 + h1 + l0}{k\|\mathbf{r}_{hkl^*}\|} == \frac{1}{\|\mathbf{r}_{hkl^*}\|}$$

$$d(hkl) = \frac{\mathbf{c}}{l} \cdot \frac{h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*}{\|\mathbf{r}_{hkl^*}\|} = \frac{h0 + h0 + l1}{l\|\mathbf{r}_{hkl^*}\|} == \frac{1}{\|\mathbf{r}_{hkl^*}\|}$$

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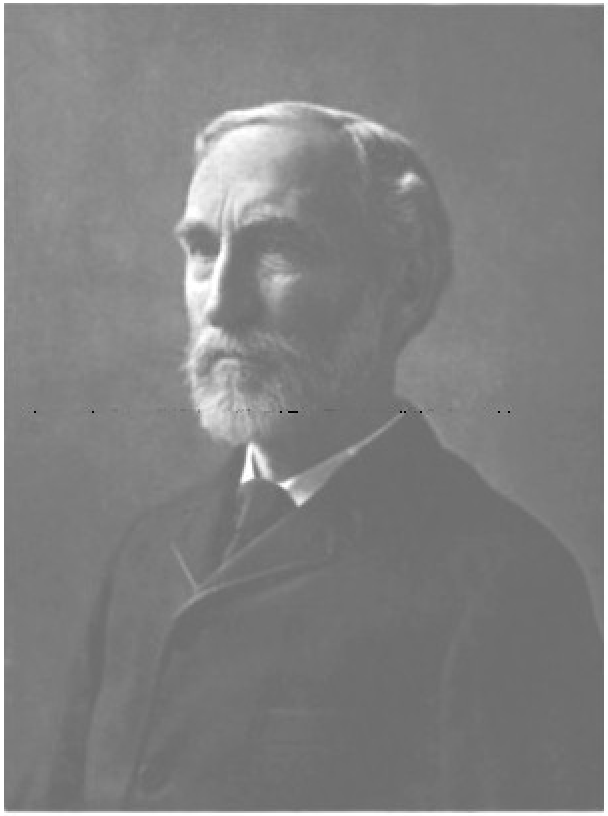
Not really Ewald's discovery....



Josiah Willard Gibbs
(1839-1903)

Reciprocal system of vectors (1881)

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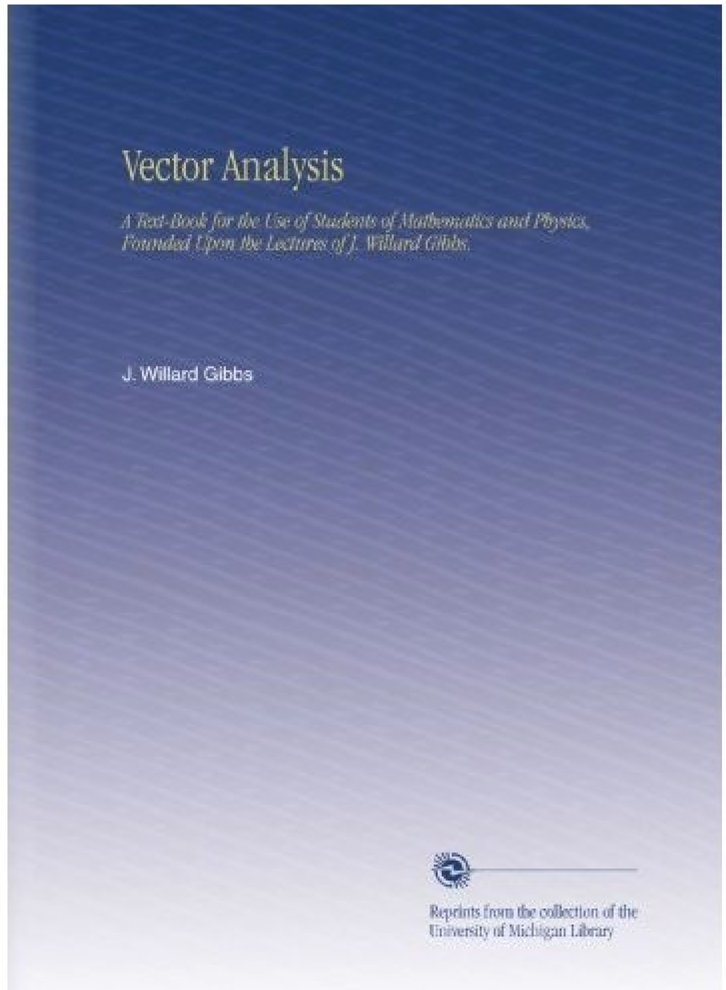
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