Indexing electron diffraction patterns

Artem Abakumov

Center for Energy Science and Technology, Skoltech

Skoltech
Skolkovo Institute of Science and Technology

Wave properties of electron

Energy of electron accelerated in the potential U:

$$E = eU = \frac{m_o v^2}{2} \Rightarrow v = \sqrt{\frac{2eU}{m_o}}$$

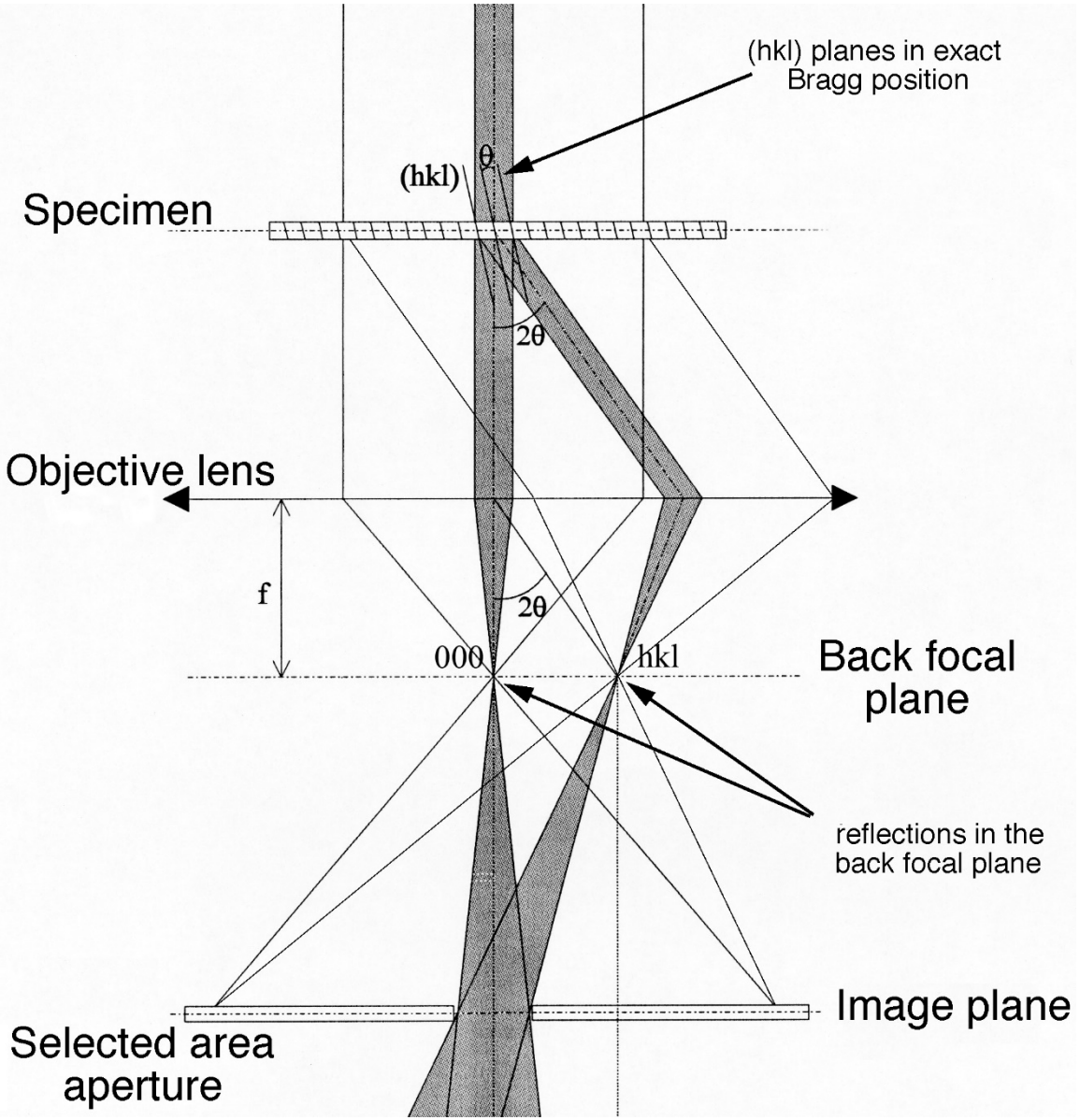
De Broglie equation: $\lambda = \frac{h}{mv} \Rightarrow \lambda = \frac{h}{\sqrt{2em_0U}} = \frac{1.226}{\sqrt{U}}$ (U in volts, λ in nm)

Relativistic correction (U > 100 kV):

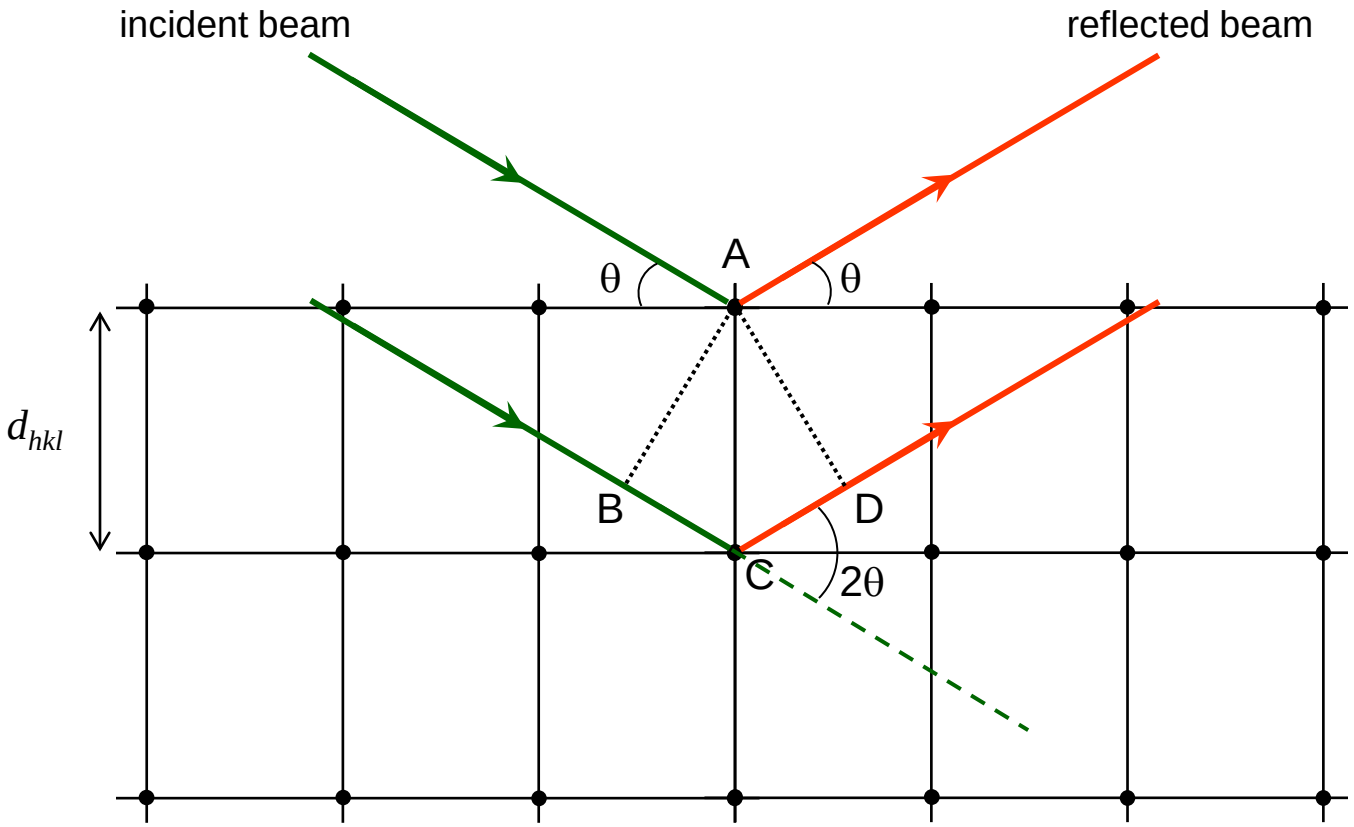
$$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}} \Rightarrow \lambda = \frac{h}{\sqrt{2m_0eU(1+\frac{eU}{2m_0c^2})}} = \frac{1.226}{\sqrt{U}}(1+9.79.10^{-7}U)^{1/2}$$

Electron energy, keV	wavelength, Å	velocity (10^8 m/s)
100	0.037	1.644
120	0.0335	1.759
200	0.0251	2.086
300	0.0197	2.330
400	0.0164	2.484

Selected area electron diffraction (SAED)



Bragg's law



path difference:

$\delta = |BC| + |CD| = 2|AC| \sin\theta = 2d_{hkl}\sin\theta$

$2d_{hkl}\sin\theta = n\lambda$ (n – integer) - Bragg's law

$d_{hkl} = nd_{nh\ nk\ nl}$

$2d_{nh\ nk\ nl}\sin\theta = \lambda$ (n – integer) – n^{th} order reflection from ($h\ k\ l$) coincides with 1st order reflection from ($nh\ nk\ nl$)

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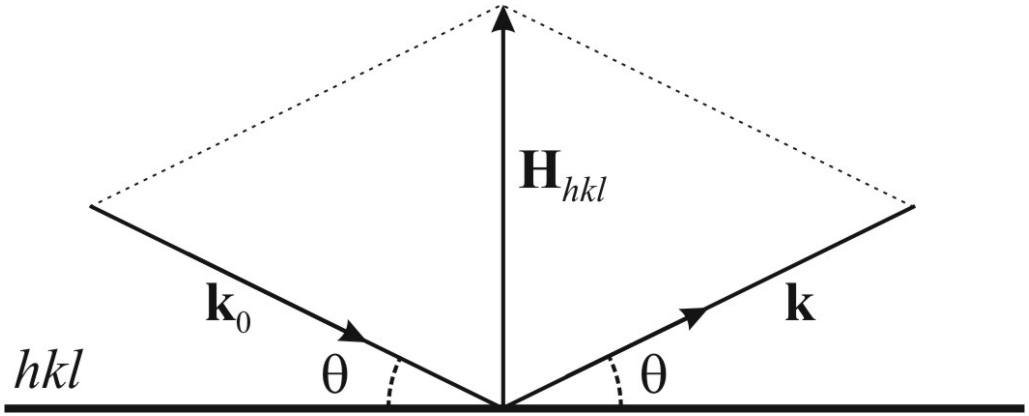
Reciprocal lattice



a* ⊥ **bc** plane

b* ⊥ **ac** plane

c* ⊥ **ab** plane

Set of the $\mathbf{H}_{hkl}$ vectors form a reciprocal lattice of crystal

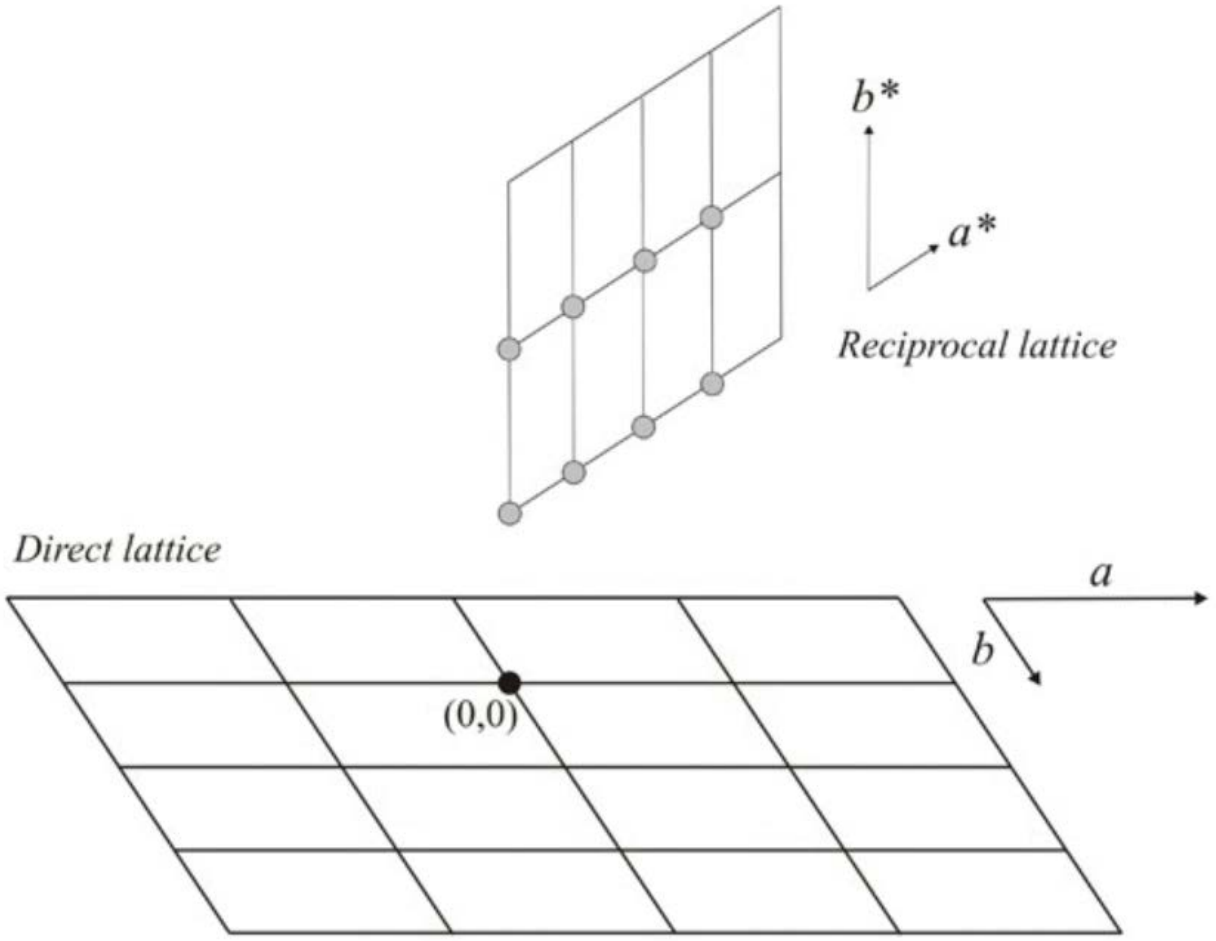
$\mathbf{k}_0$ – wave vector of the incident beam, $|\mathbf{k}_0| = 1/\lambda$

$\mathbf{k}$ – wave vector of the diffracted beam, $|\mathbf{k}| = 1/\lambda$

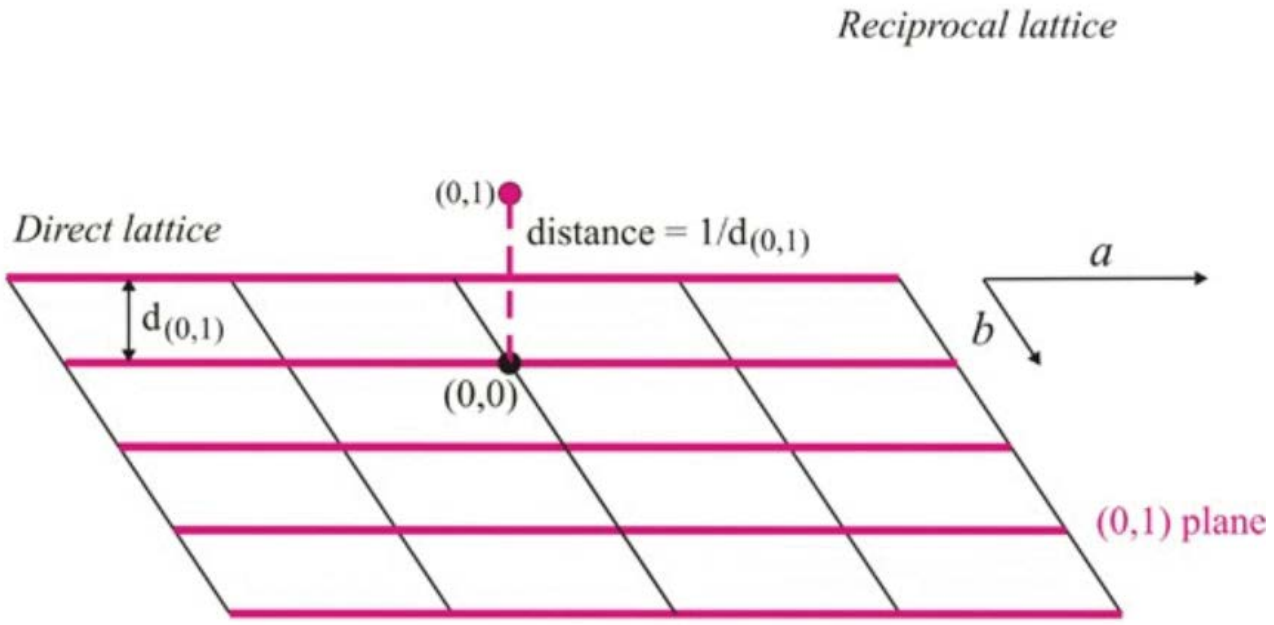
$\mathbf{H}_{hkl} \perp hkl$ plane, $\mathbf{H} = \mathbf{k} - \mathbf{k}_0$

Bragg's condition is satisfied if $|\mathbf{H}| = 2\sin\theta/\lambda = 1/d_{hkl}$

Reciprocal lattice



Reciprocal lattice



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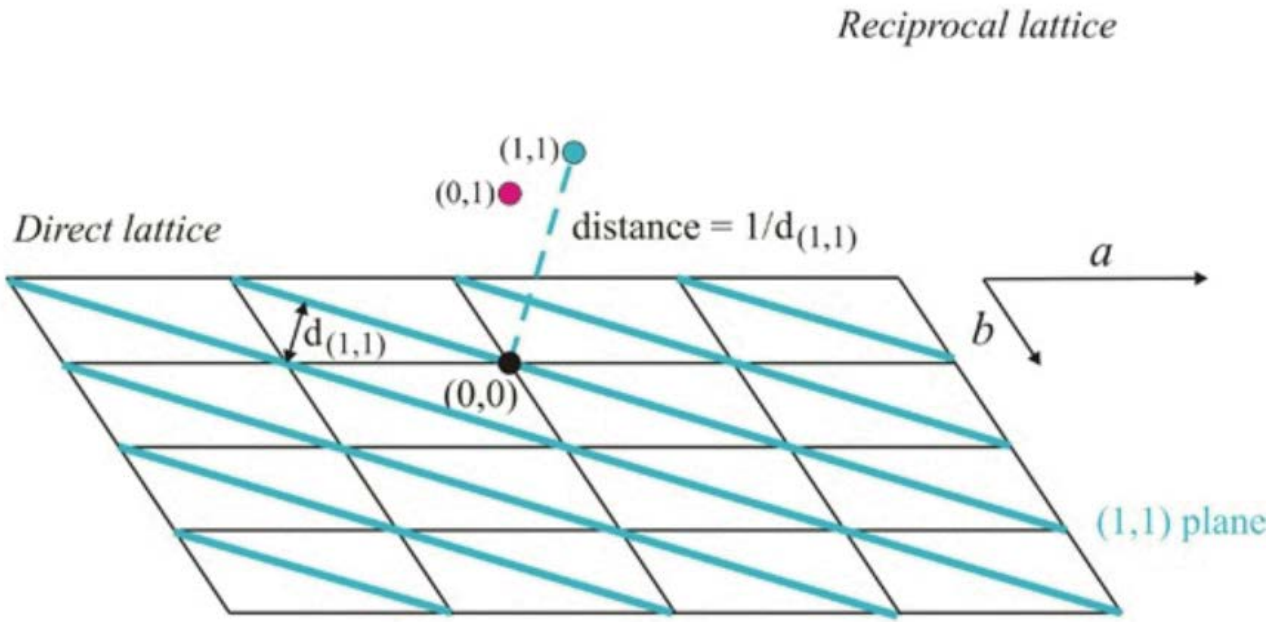

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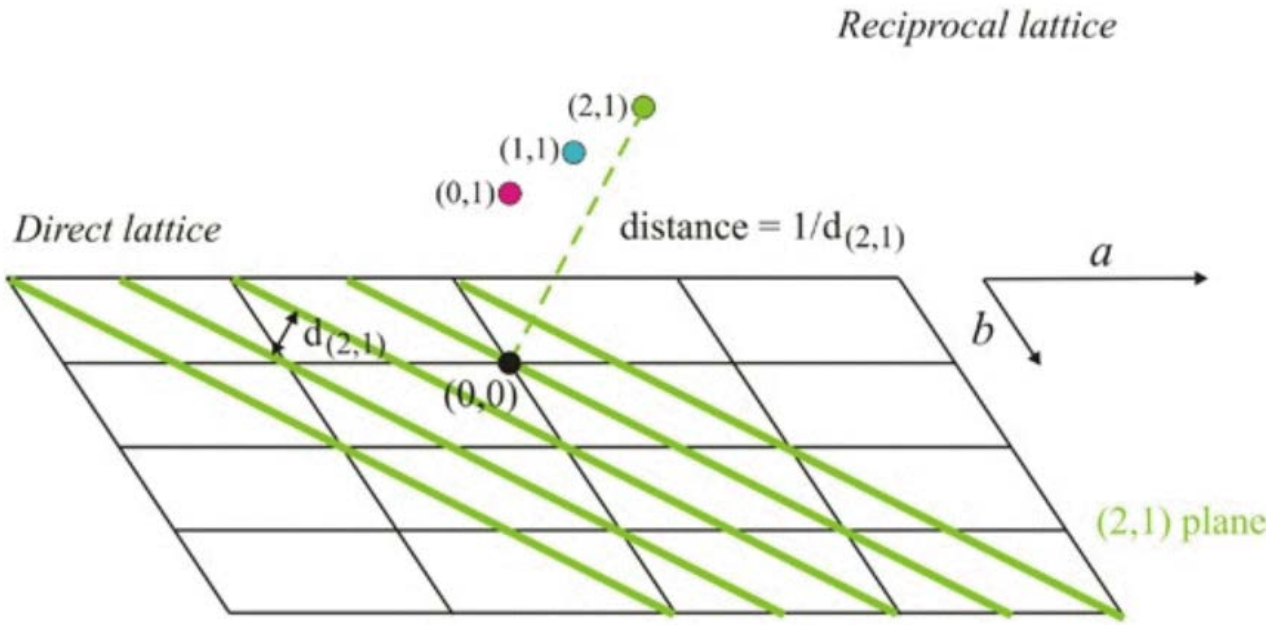

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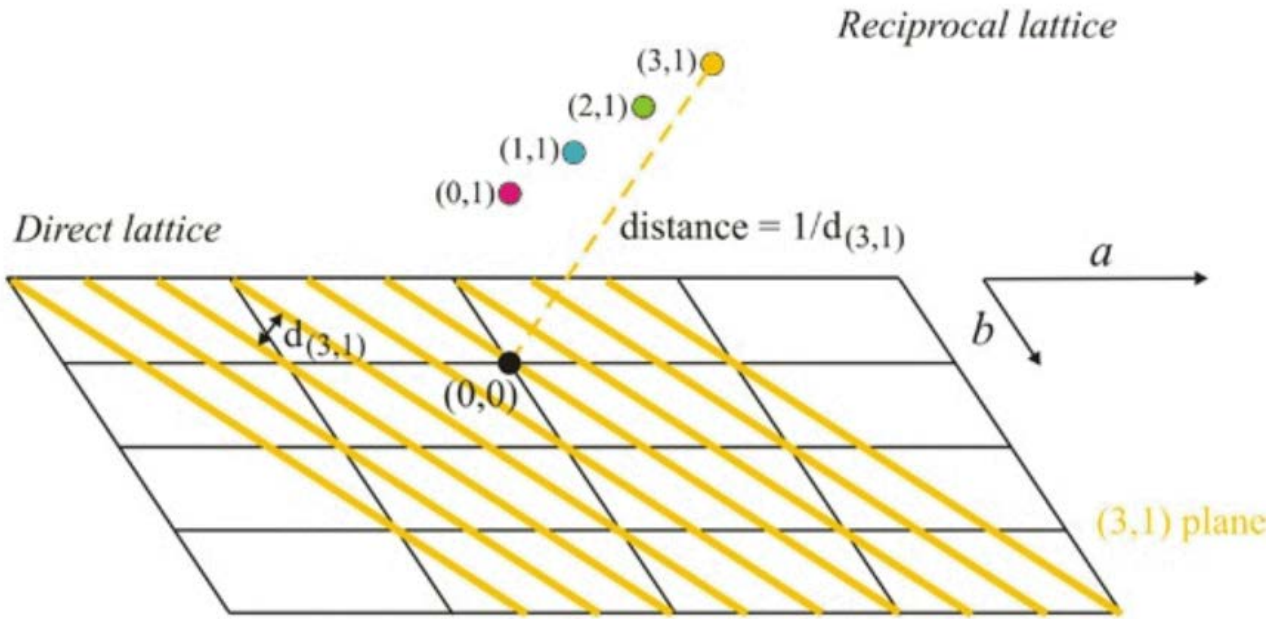
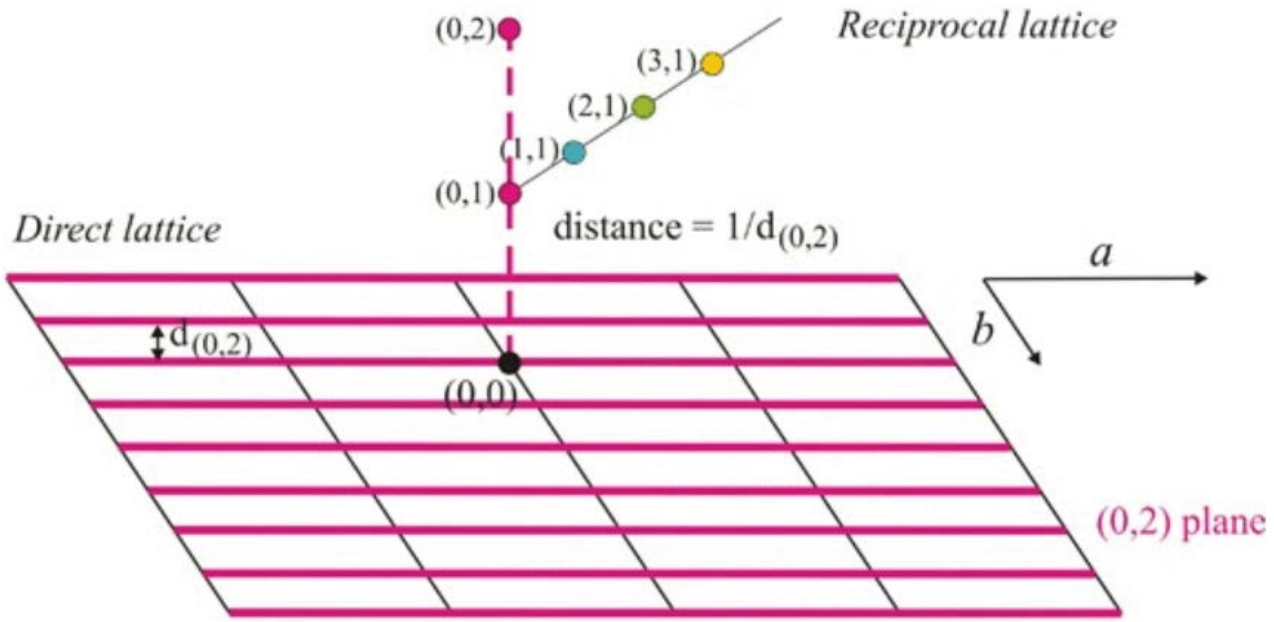
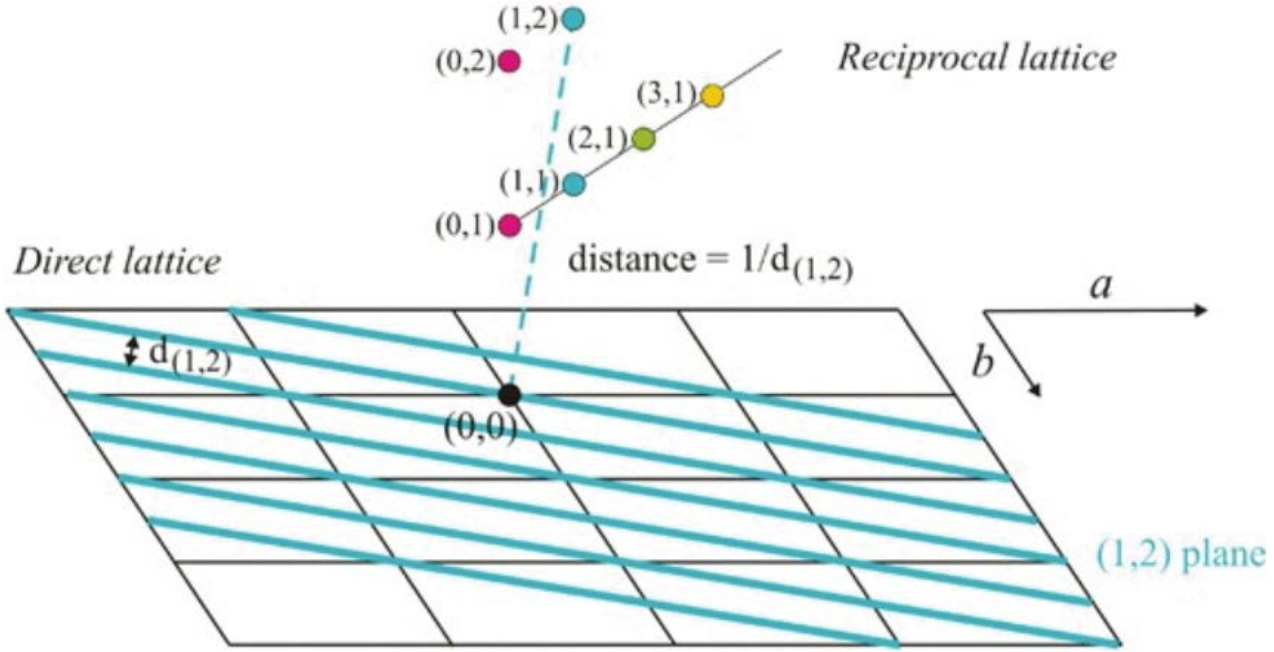


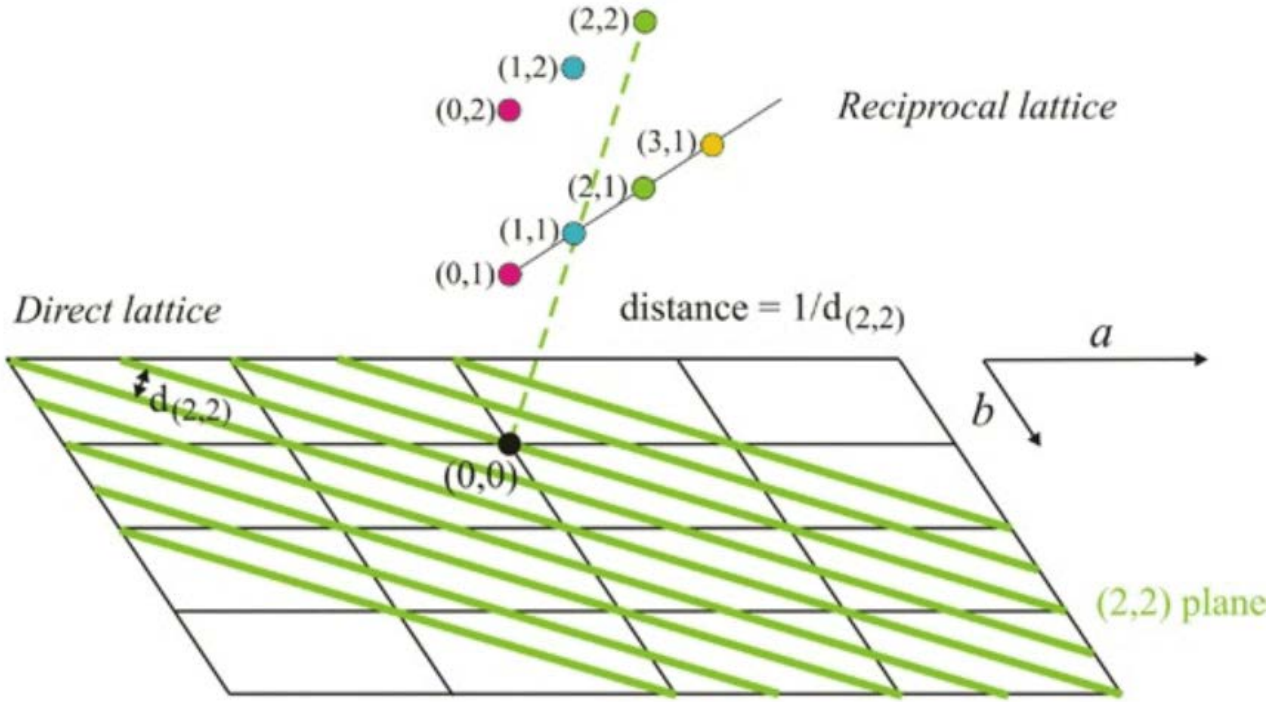
Reciprocal lattice



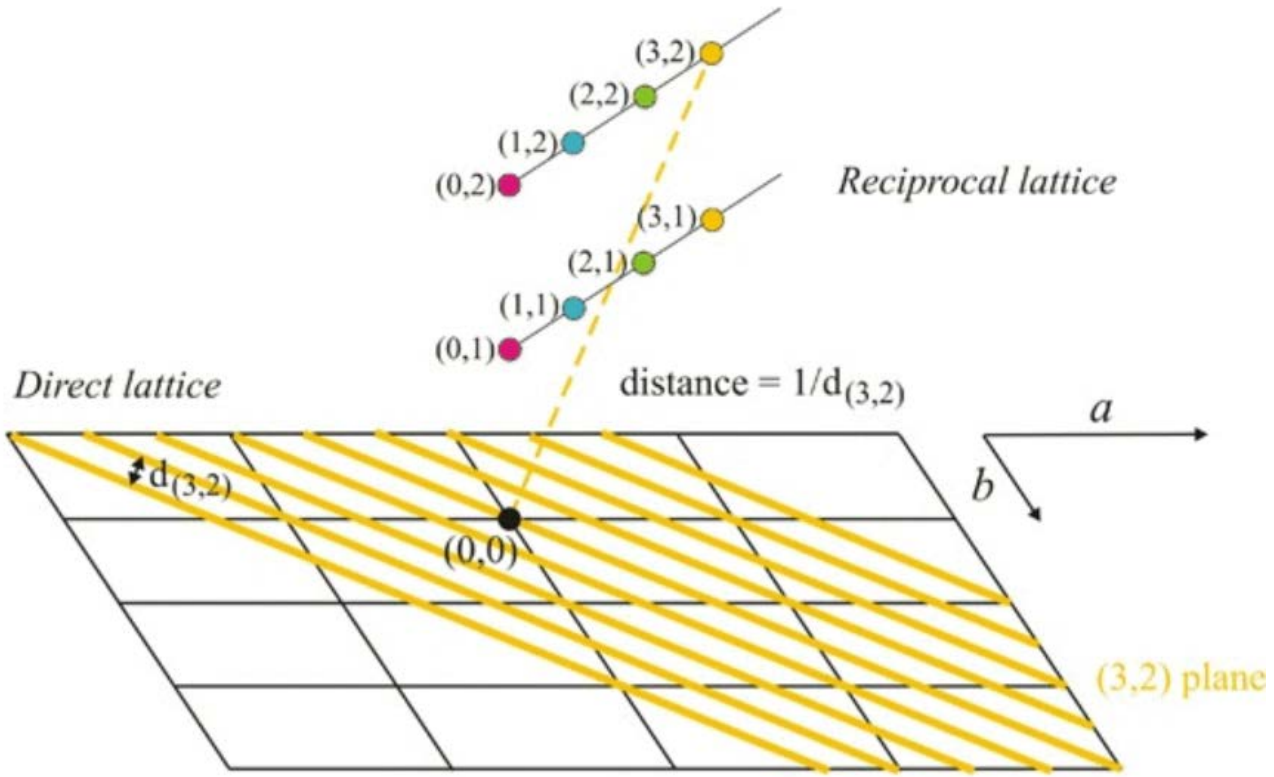
Reciprocal lattice



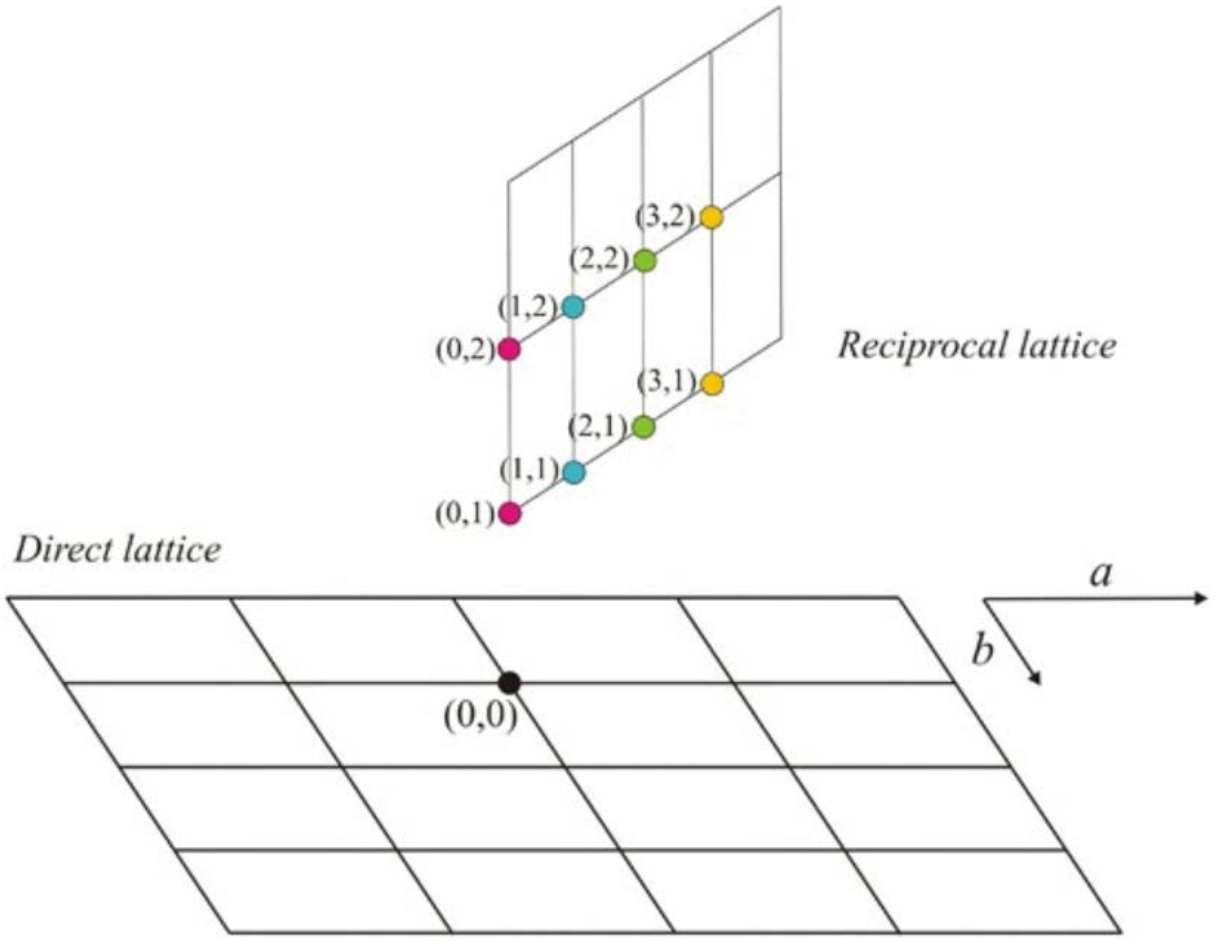
Reciprocal lattice



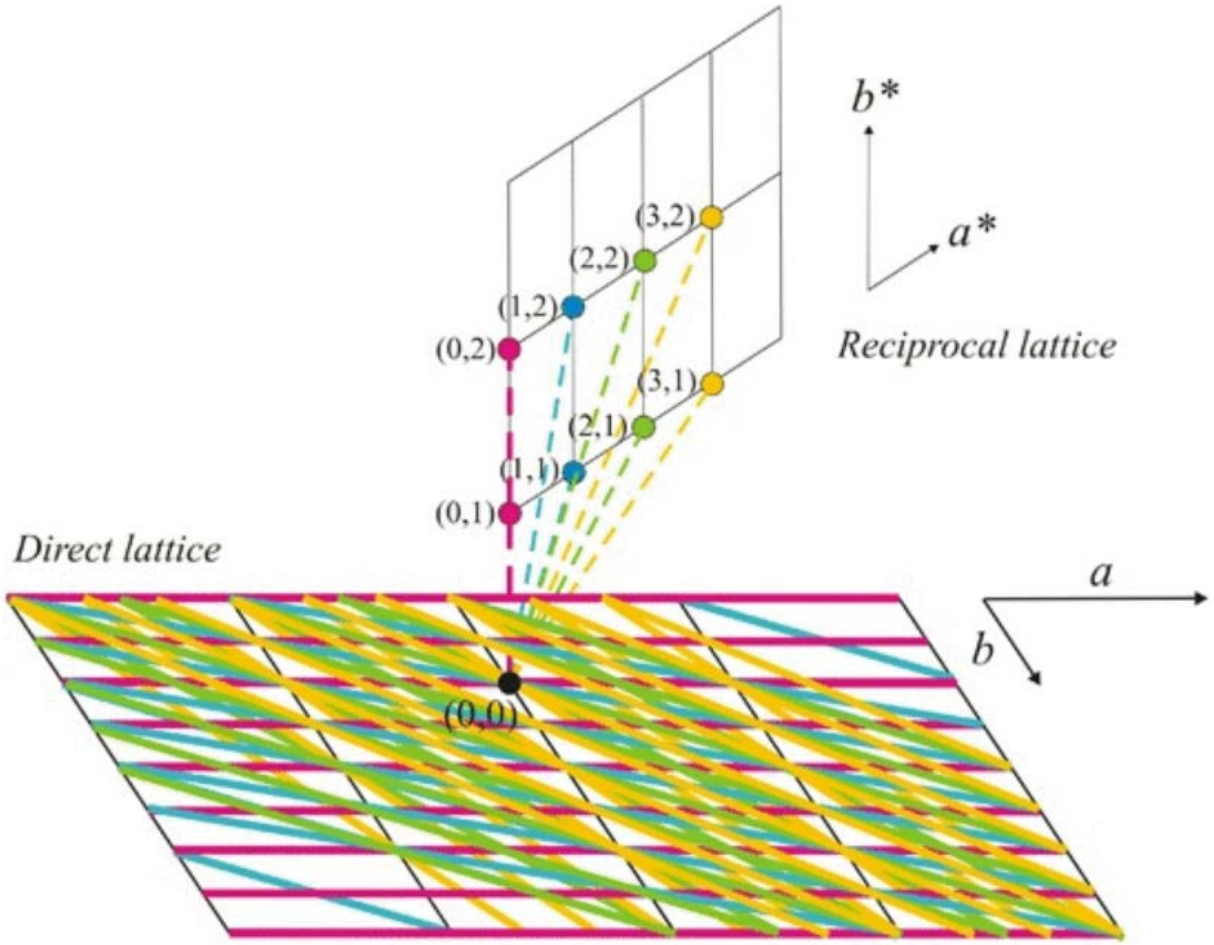
Reciprocal lattice



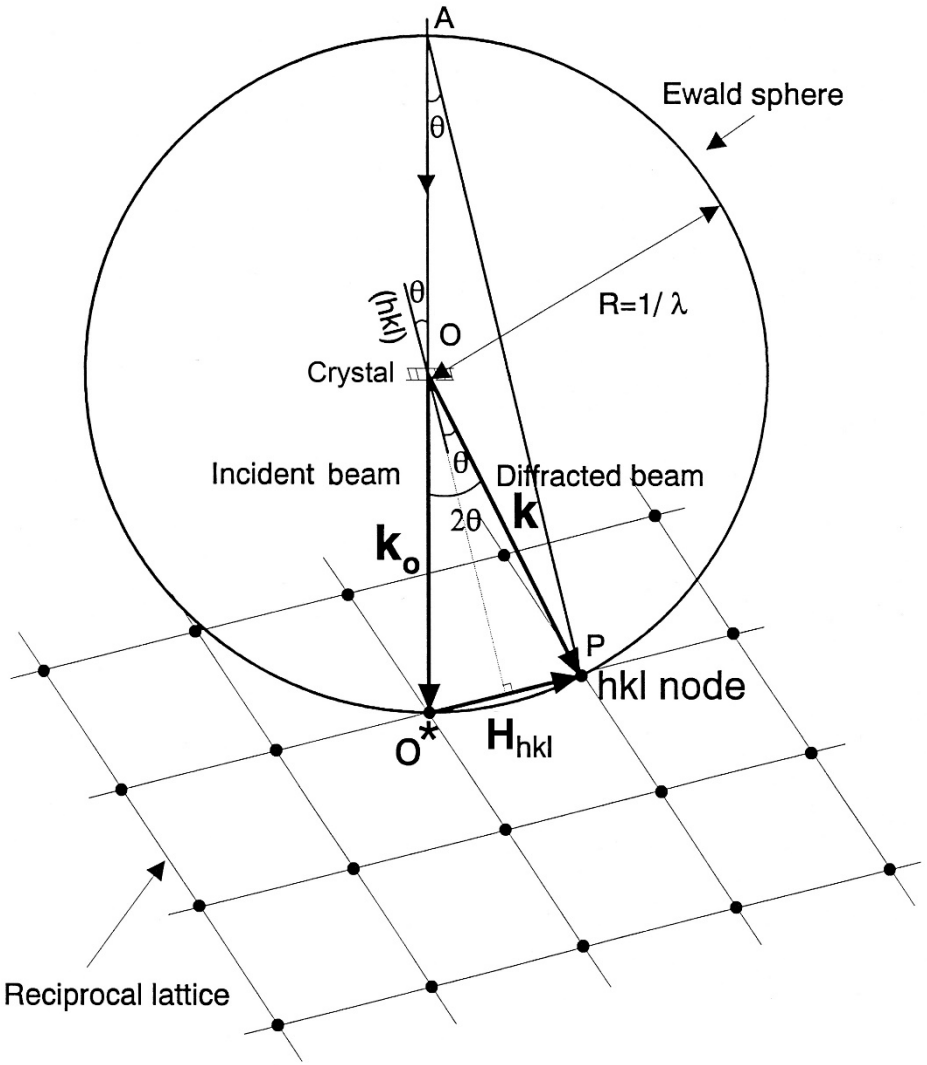
Reciprocal lattice



Reciprocal lattice

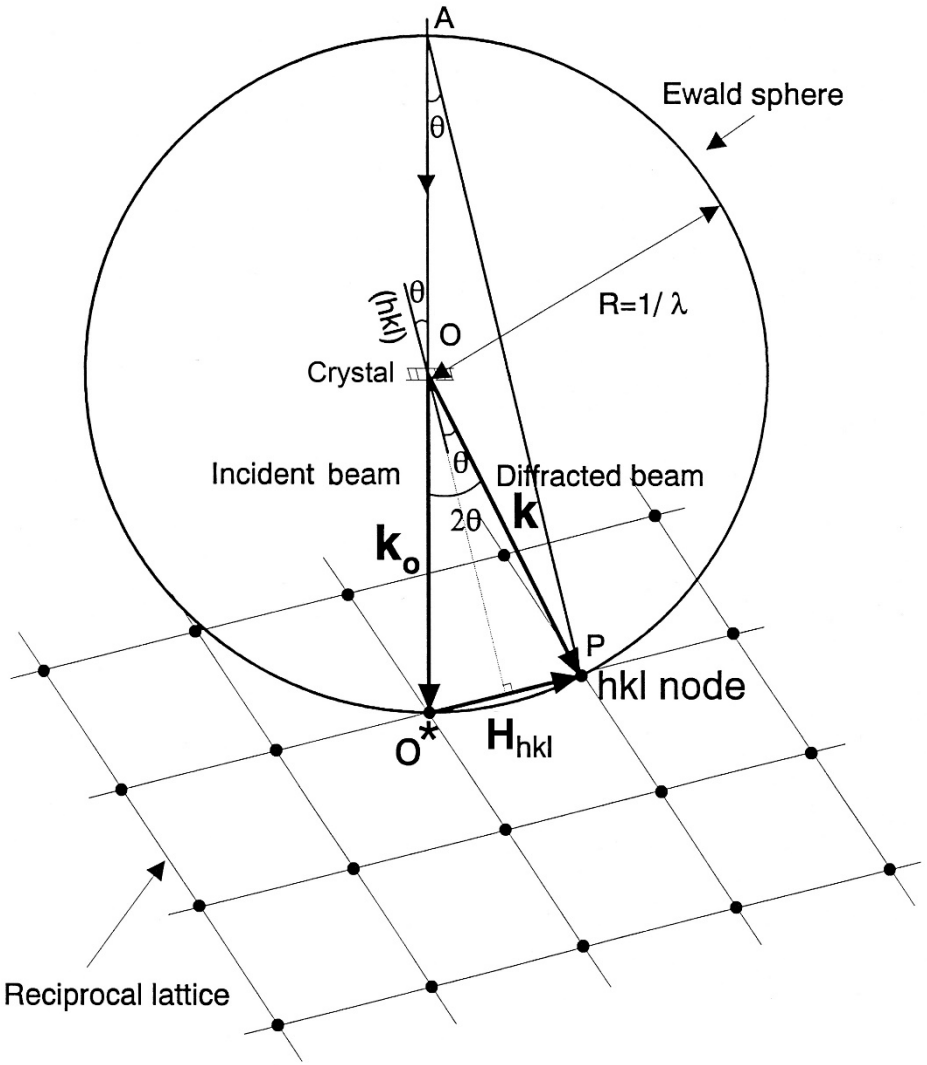


Reciprocal lattice and the Ewald sphere



1. Draw an Ewald sphere with the radius of $1/\lambda$
2. Place the crystal at the center of the sphere
3. Draw the incident beam wavevector $\mathbf{k}_0$ from the center of the sphere
4. Place the origin of the reciprocal lattice O* at the intersection of the Ewald sphere and $\mathbf{k}_0$
5. Rotate the crystal and reciprocal lattice to place *hkl* reciprocal lattice node on the Ewald sphere
6. The wavevector of the diffracted beam **k** connects the center of the sphere and the *hkl* node

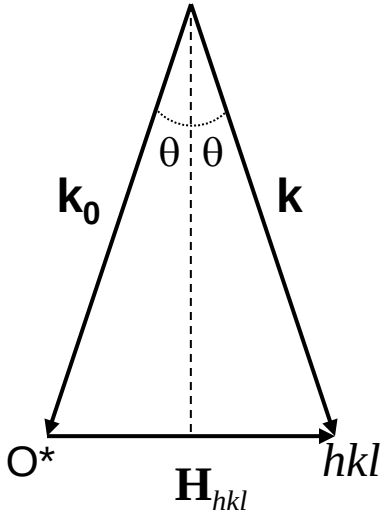
Reciprocal lattice and the Ewald sphere



$\angle \mathbf{k},\mathbf{k}_0 = 2\theta$

$|\mathbf{H}_{hkl}| = 1/d_{hkl}$

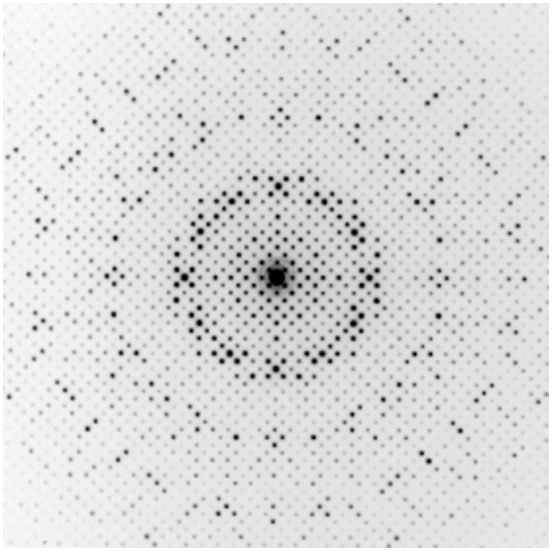
$|\mathbf{k}| = |\mathbf{k}_0| = 1/\lambda$



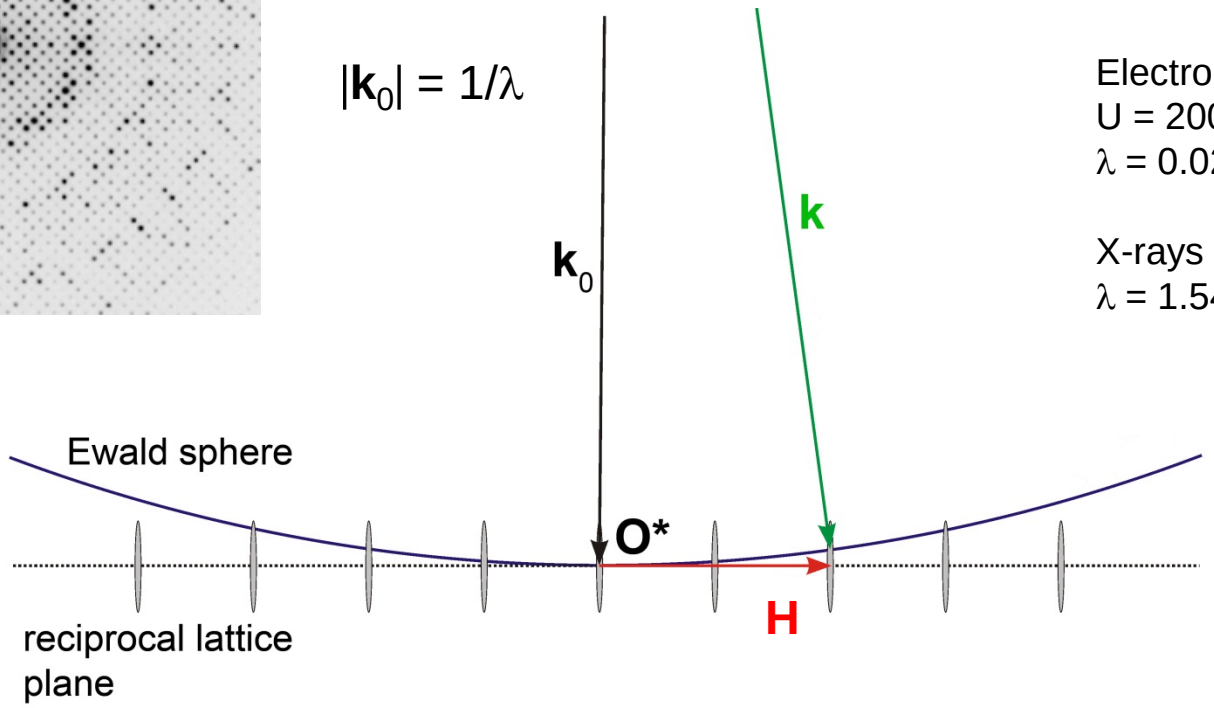
$|\mathbf{H}_{hkl}| = 2|\mathbf{k}_0| sin\theta$

$1/d_{hkl} = 2/\lambda \sin\theta$

Selected area electron diffraction (SAED)



$$\lambda = \frac{h}{\sqrt{2em_0 U}} = \frac{12.26}{\sqrt{U}}$$



Electrons:
U = 200kV
λ = 0.027Å

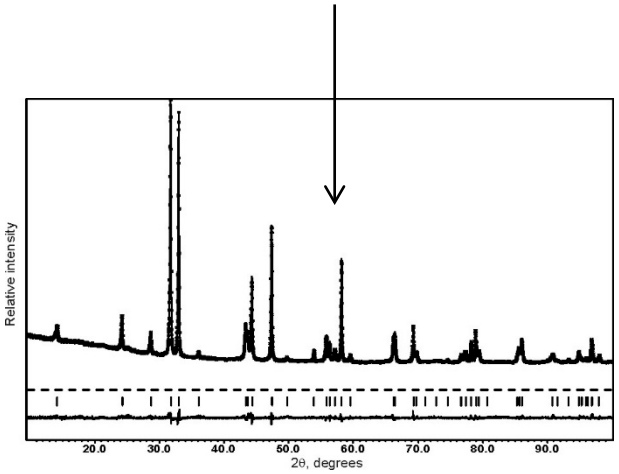
X-rays ($CuK_{\alpha 1}$)
λ = 1.5406Å

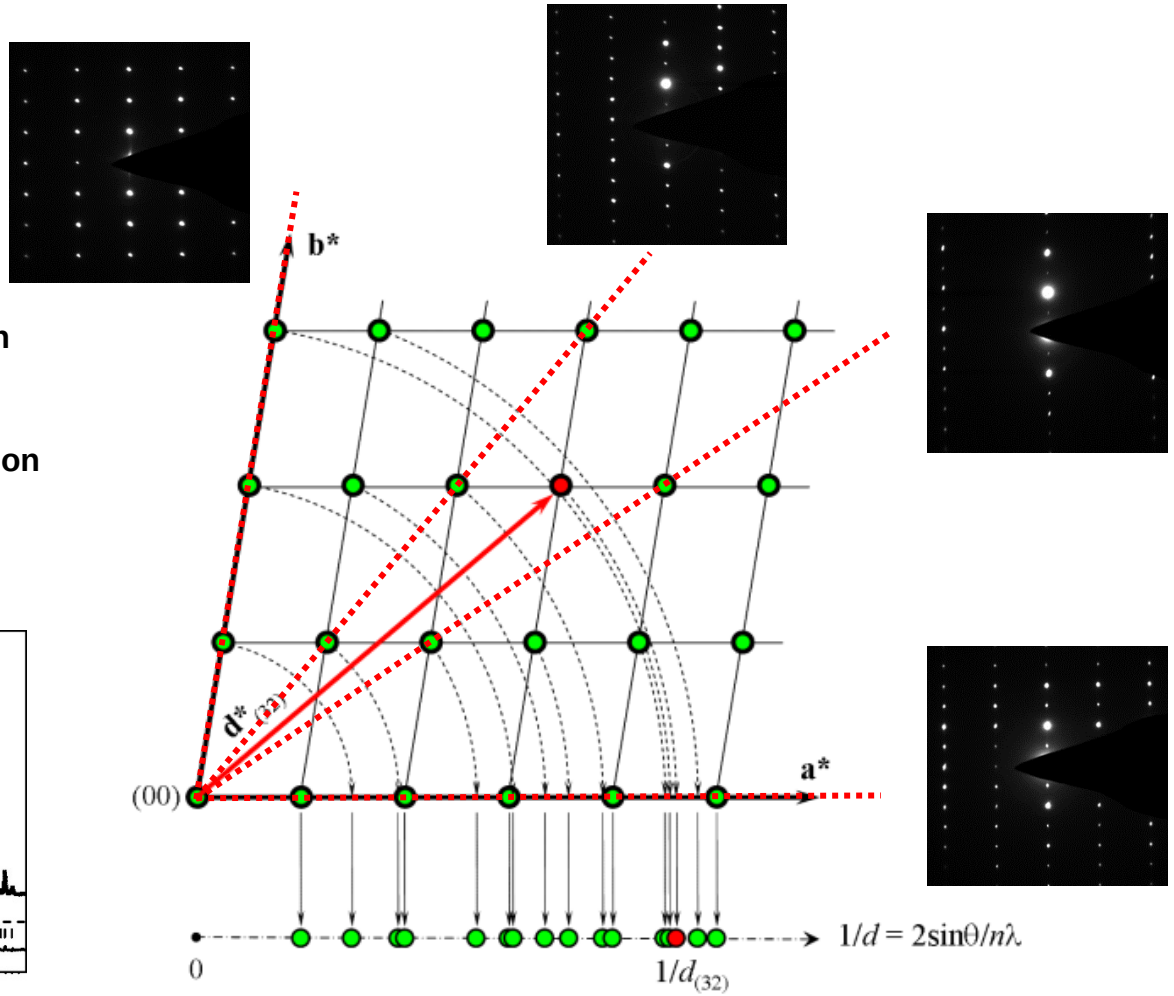
Electron diffraction pattern is a section of the reciprocal lattice of a crystal

SAED vs PXRD

Electron diffraction pattern: 2D section of the 3D reciprocal lattice

Powder diffraction pattern: 1D projection of the 3D reciprocal lattice

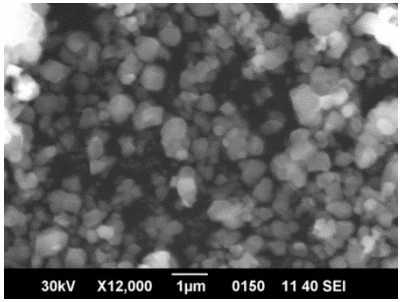


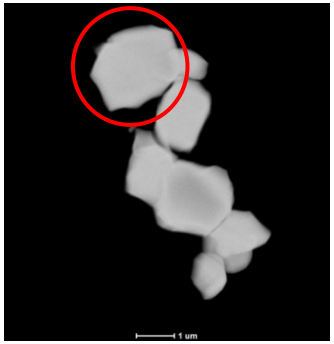


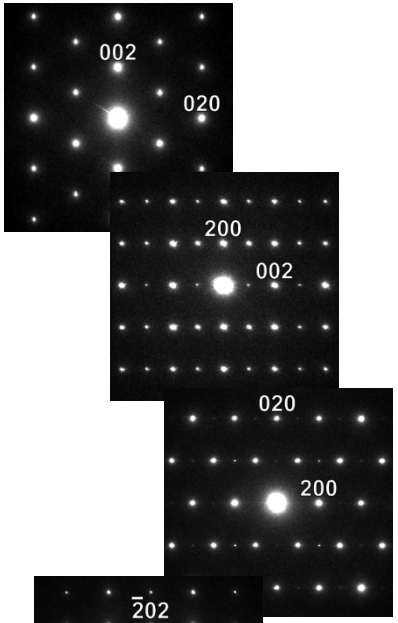
SAED and PXRD

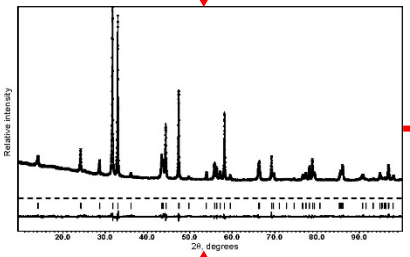
Polycrystalline sample

Crystallites

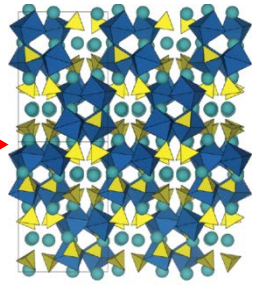






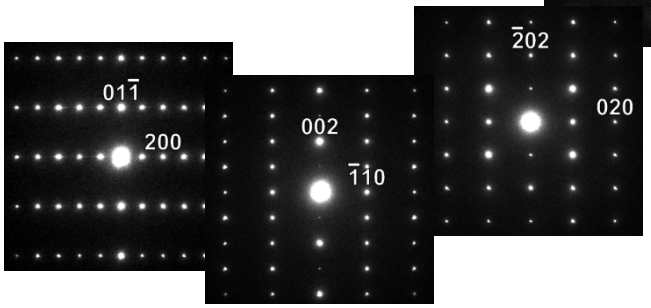


Structure solution
Rietveld refinement



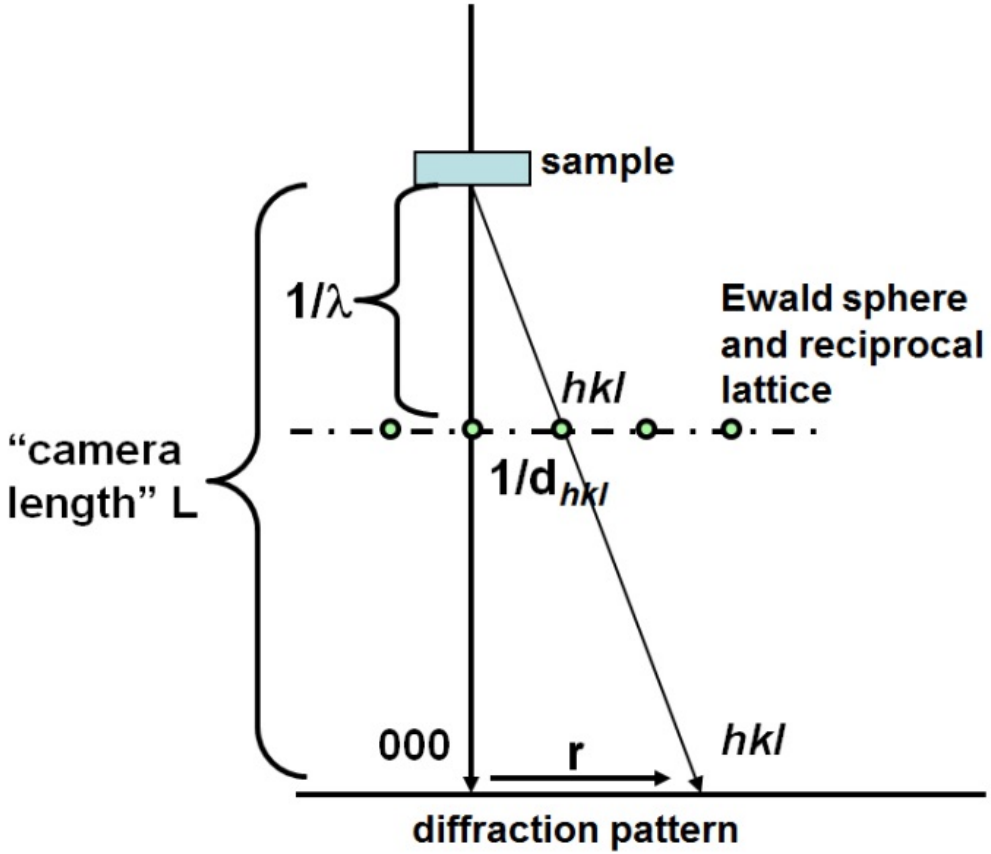
Unit cell parameters
Space group

Electron diffraction patterns



SAED: interplanar spacings

Bragg equation for electron diffraction:



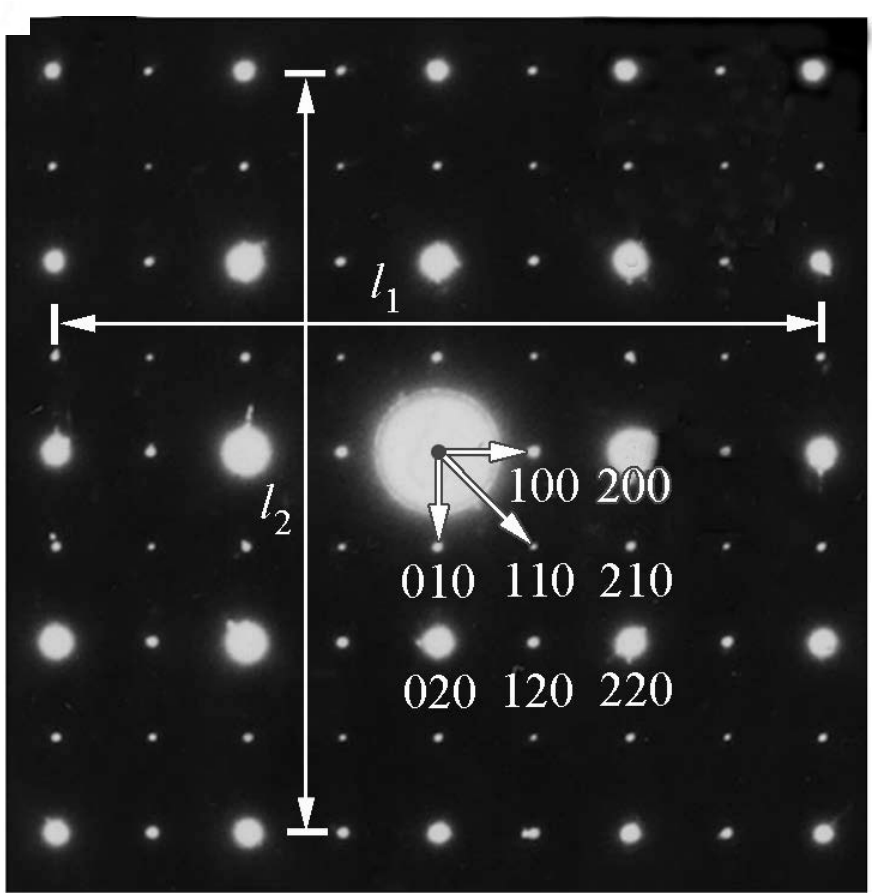
$$\left|\mathbf{H}_{hkl}\right|\lambda = r / L$$

$$\left|\mathbf{H}_{hkl}\right| = \frac{1}{d_{hkl}}$$

$$d_{hkl} = \lambda L / r$$

$\mathbf{H}_{hkl}$ – reciprocal lattice vector

SAED: interplanar spacings



Interplanar spacings:

$$d_{hkl} = \frac{L\lambda}{r},\ r_i = l_i/n_i$$

$$\Downarrow$$

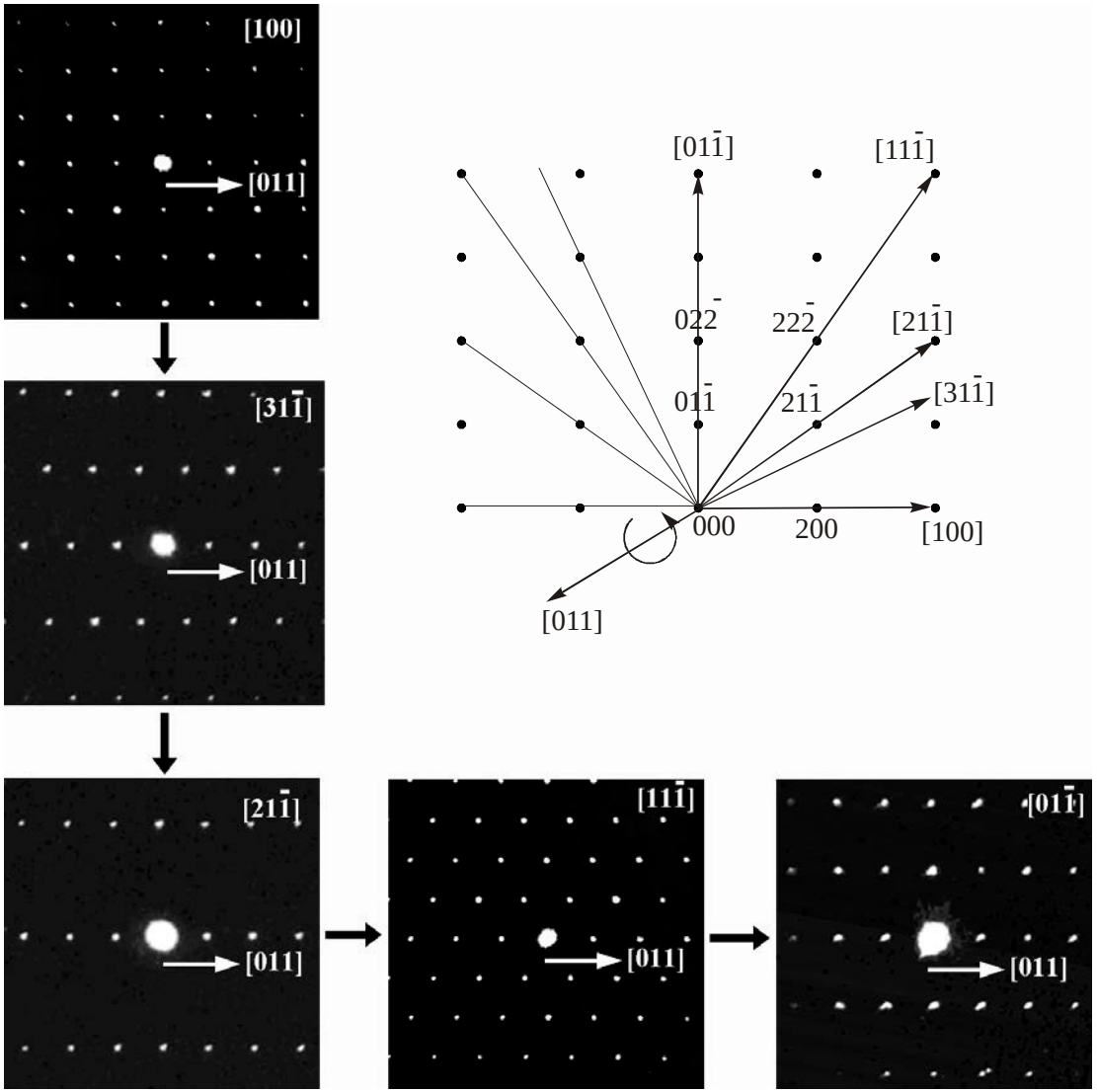
$$d_{hkl} = \frac{L\lambda n_i}{l_i}$$

zone index [*uvw*]:
two non-collinear g-vectors
$h_1k_1l_1$, $h_2k_2l_2$ (counter-clockwise):

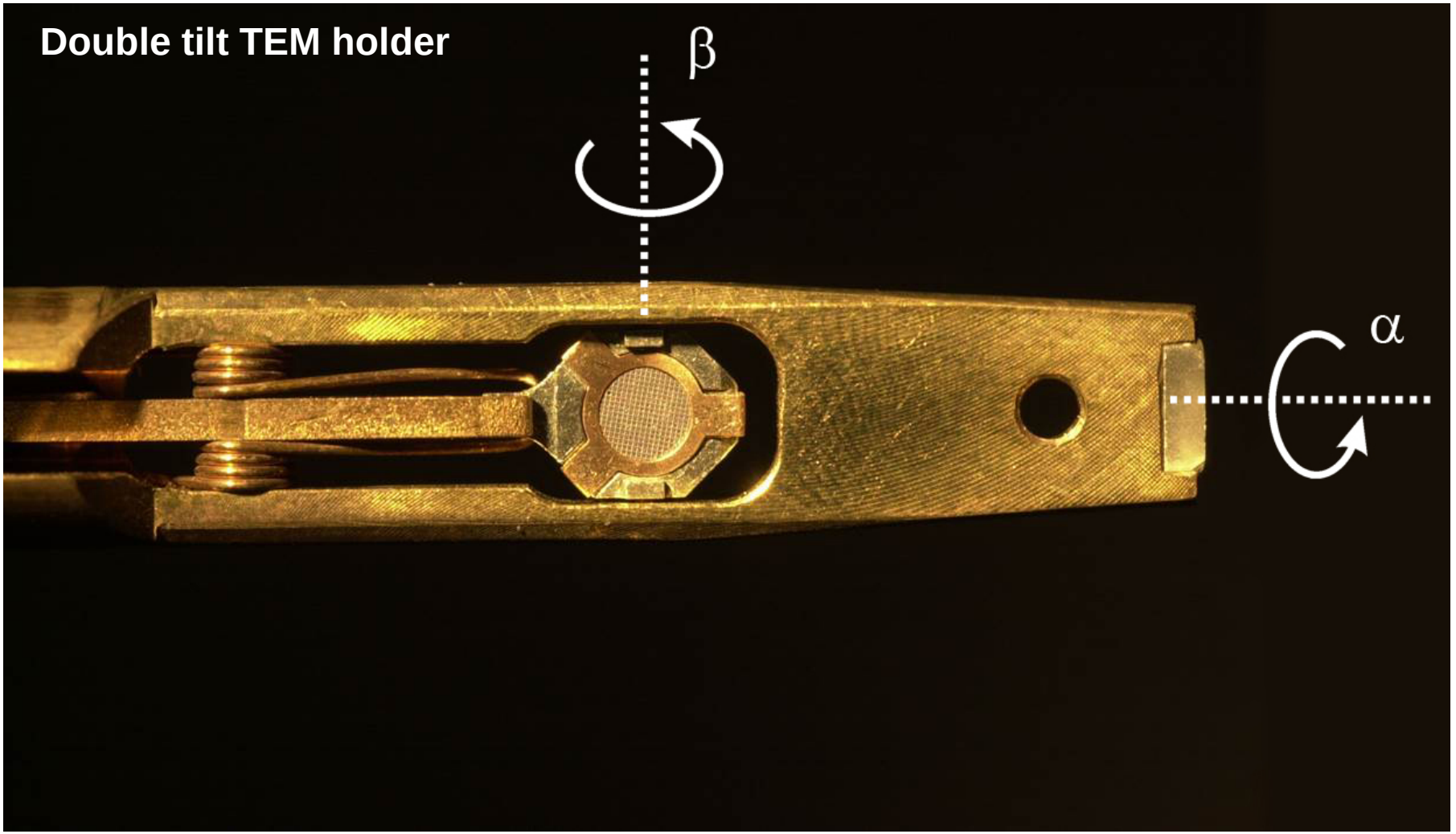
$$u = k_1l_2 - k_2l_1$$
$$v = l_1h_2 - l_2h_1$$
$$w = h_1k_2 - h_2k_1$$

Reconstruction of reciprocal lattice

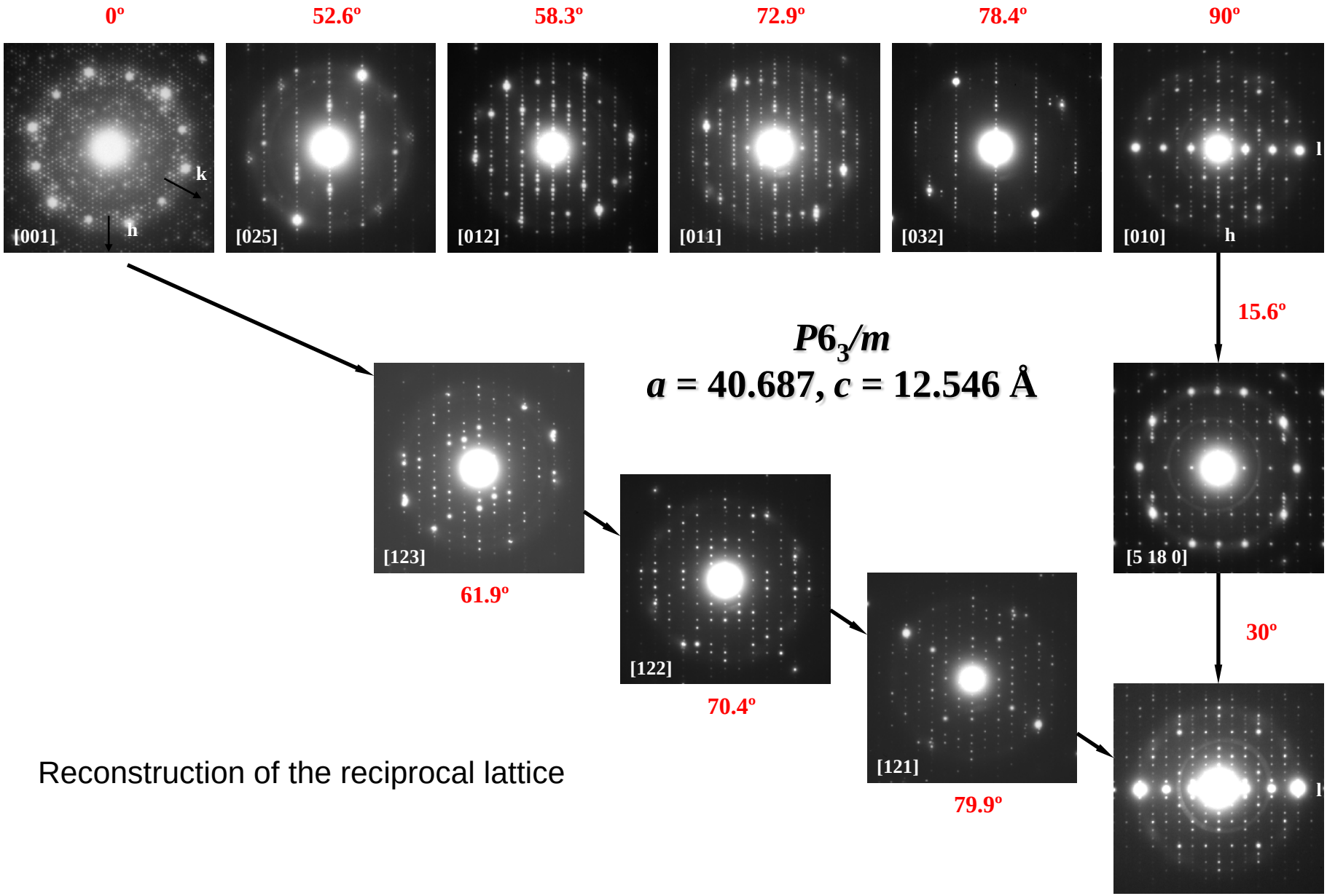
Reconstruction of the reciprocal lattice:



Reconstruction of reciprocal lattice



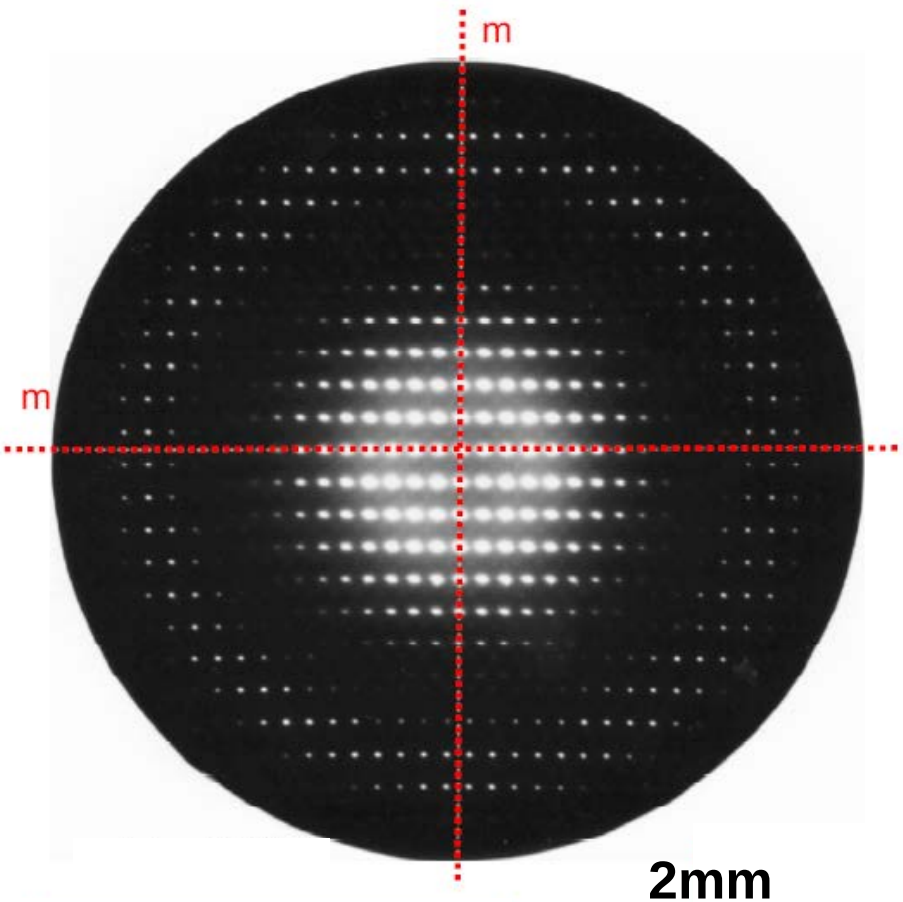
Reconstruction of reciprocal lattice

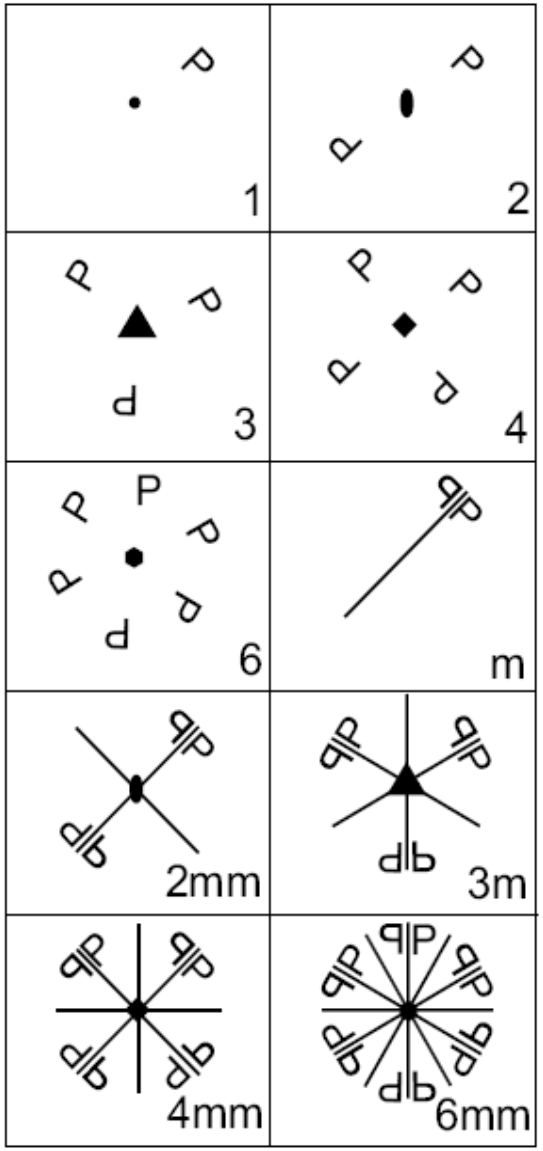


Reconstruction of the reciprocal lattice

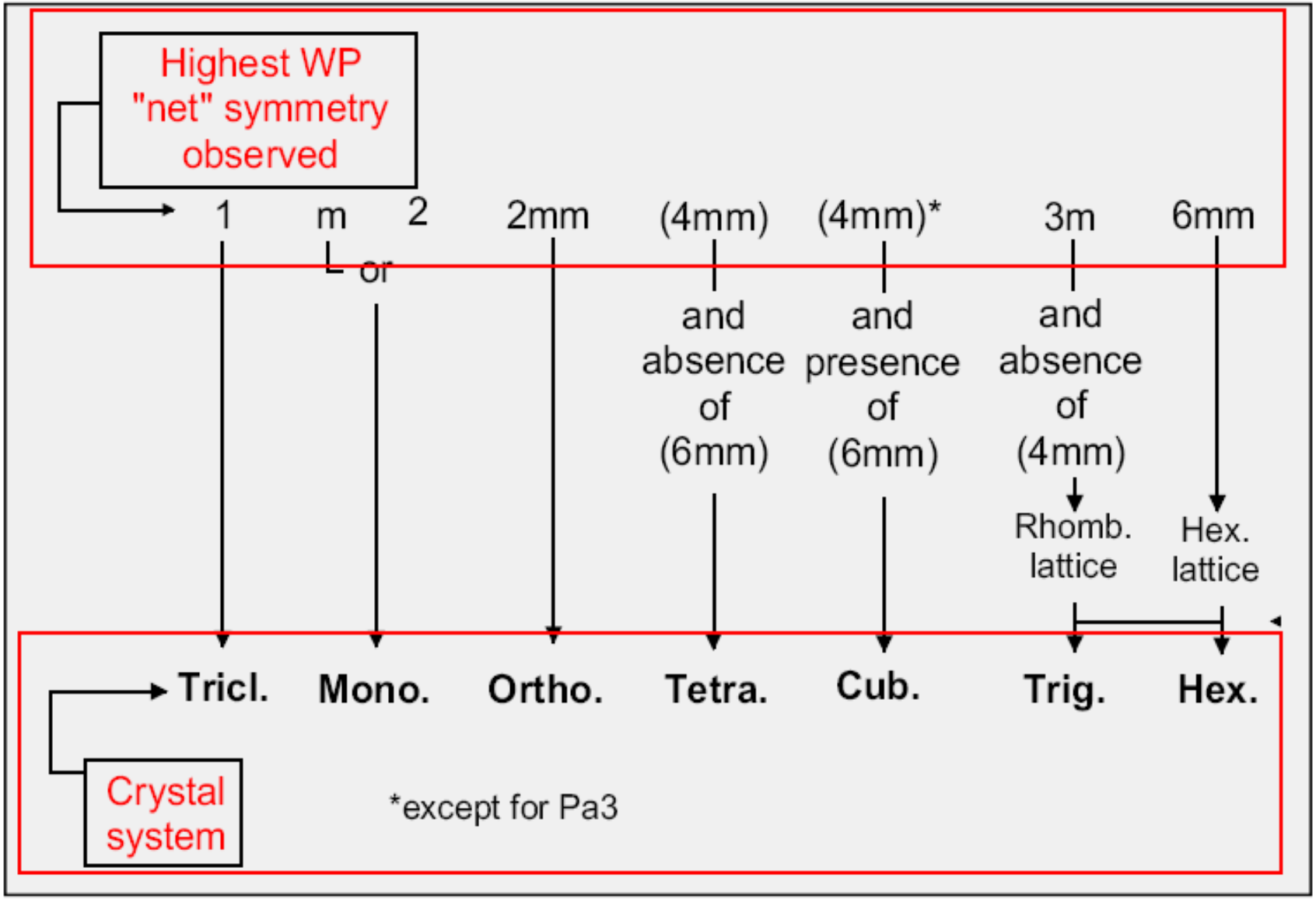
SAED: symmetry analysis

The symmetry of the SAED pattern is described by one of 10 2D point groups





SAED: symmetry analysis



From J.P. Morniroli and J.W. Steeds, Ultramicroscopy, 1992, 45, 219

Thank you for your cooperation!