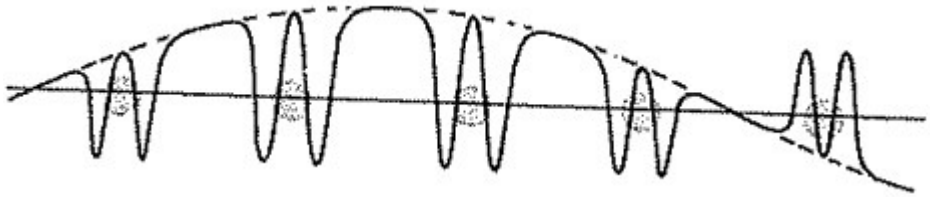
Теорема Блоха

$$H\psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right) \psi = \mathcal{E}\psi \qquad U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r})$$

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$



$$\psi_{n\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \text{ де } u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

$$\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \psi(\mathbf{r})$$

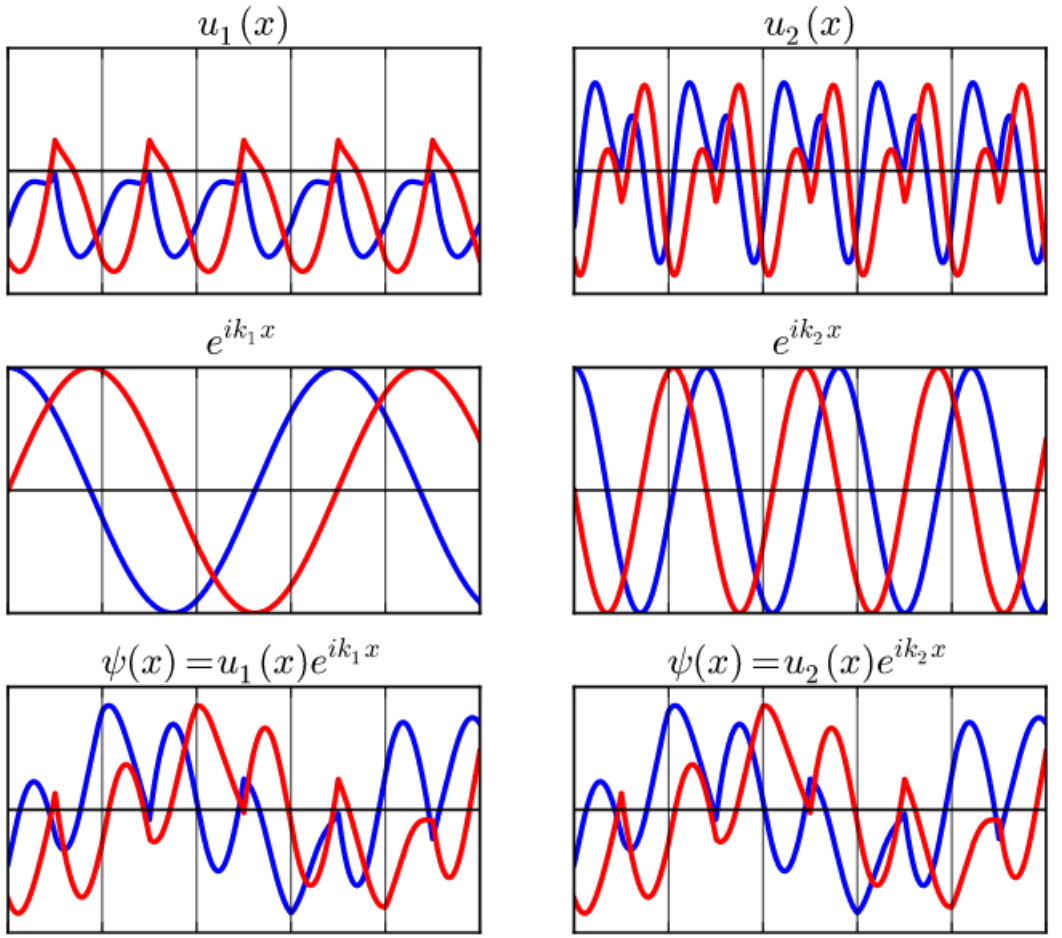
Теорема Блоха

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$

$$\psi_{n,\,\mathbf{k}+\mathbf{K}}(\mathbf{r}) = \psi_{n\mathbf{k}}(\mathbf{r})$$

$$\mathscr{E}_{n,\,\mathbf{k}+\mathbf{K}} = \mathscr{E}_{n\mathbf{k}}$$

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\,\nabla_{\mathbf{k}}\mathscr{E}_n(\mathbf{k})$$



Обернена ґратка

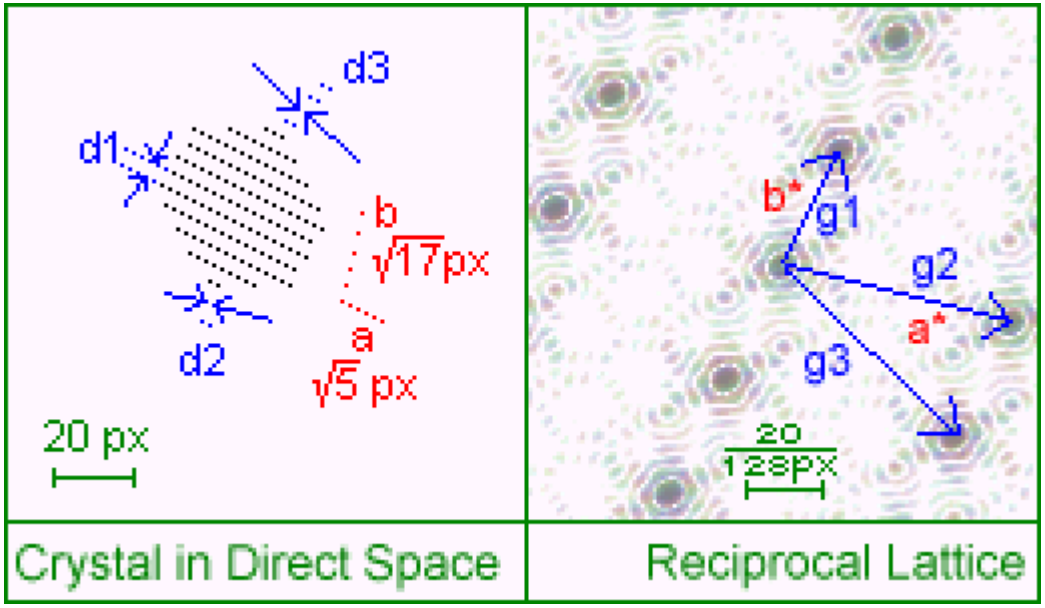
$$e^{i\boldsymbol{K}(\boldsymbol{r}+\boldsymbol{R})} = e^{i\boldsymbol{K}\boldsymbol{r}} \quad \rightarrow \quad e^{i\boldsymbol{K}\boldsymbol{R}} = 1$$

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

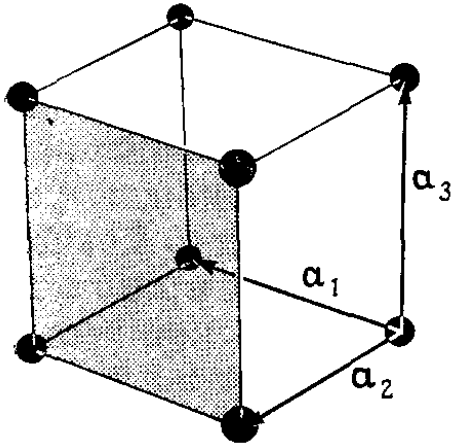
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

$$\boldsymbol{b}_i \boldsymbol{a}_j = 2\pi \delta_{ij}$$

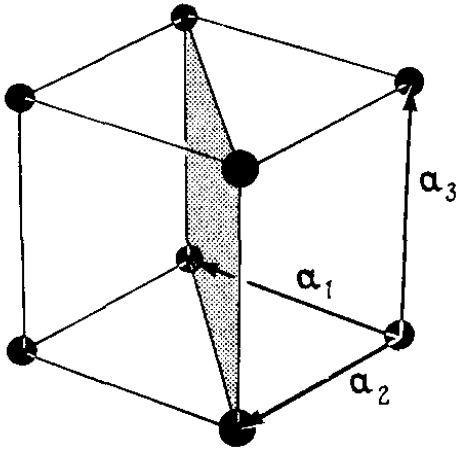


https://en.wikipedia.org/wiki/Reciprocal_lattice

Індекси Міллєра



(010)



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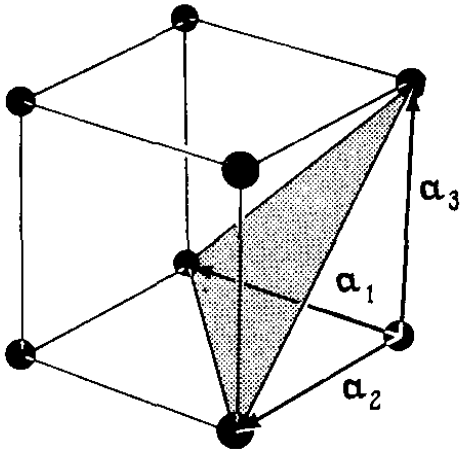

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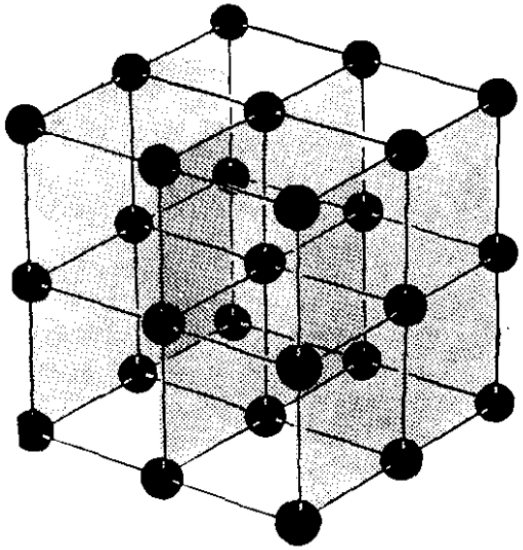
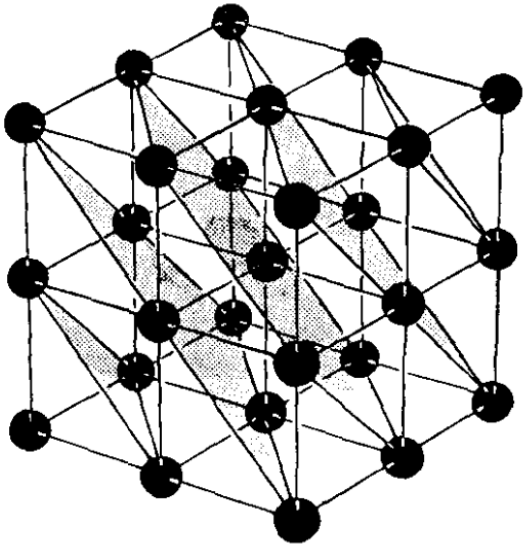
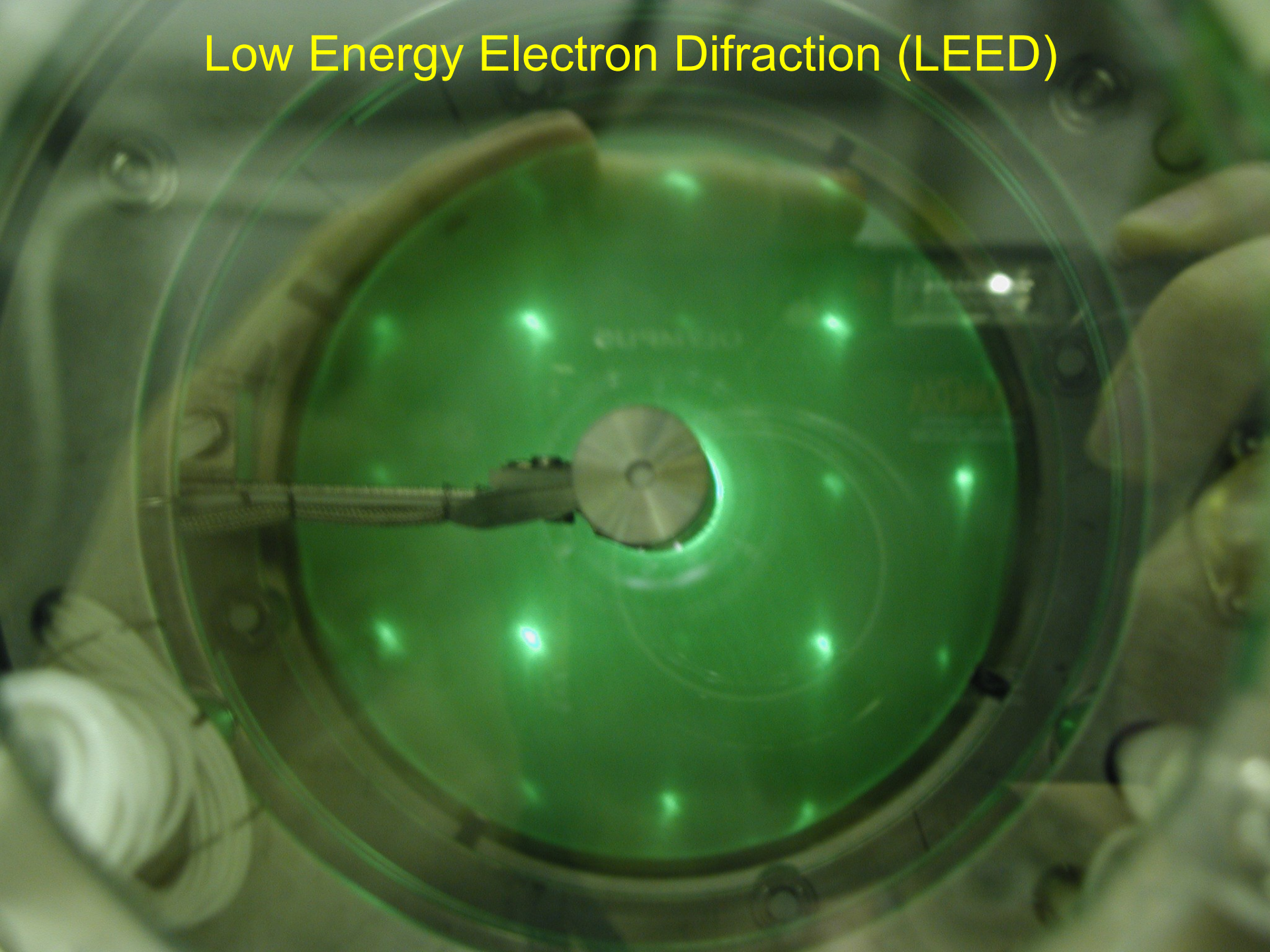
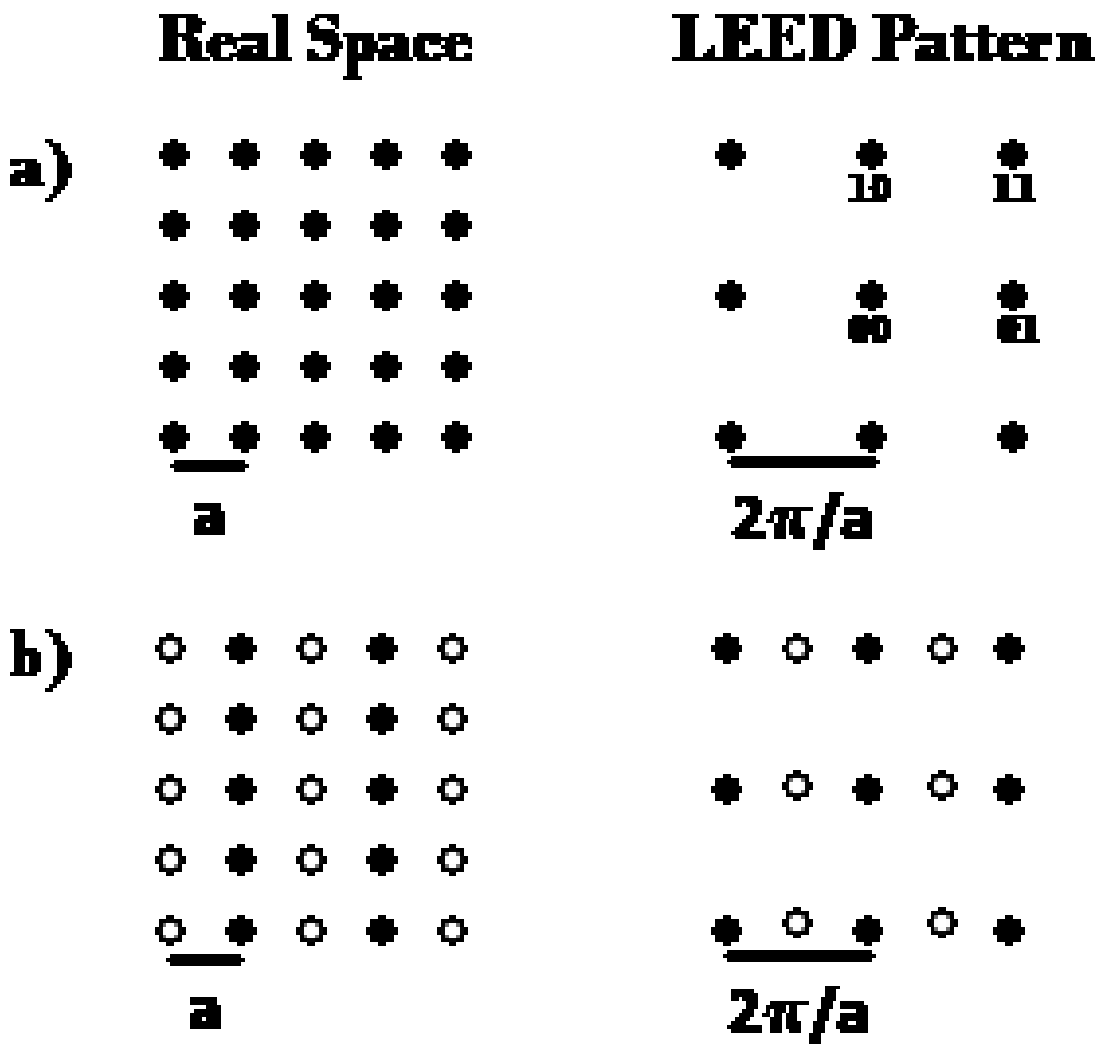
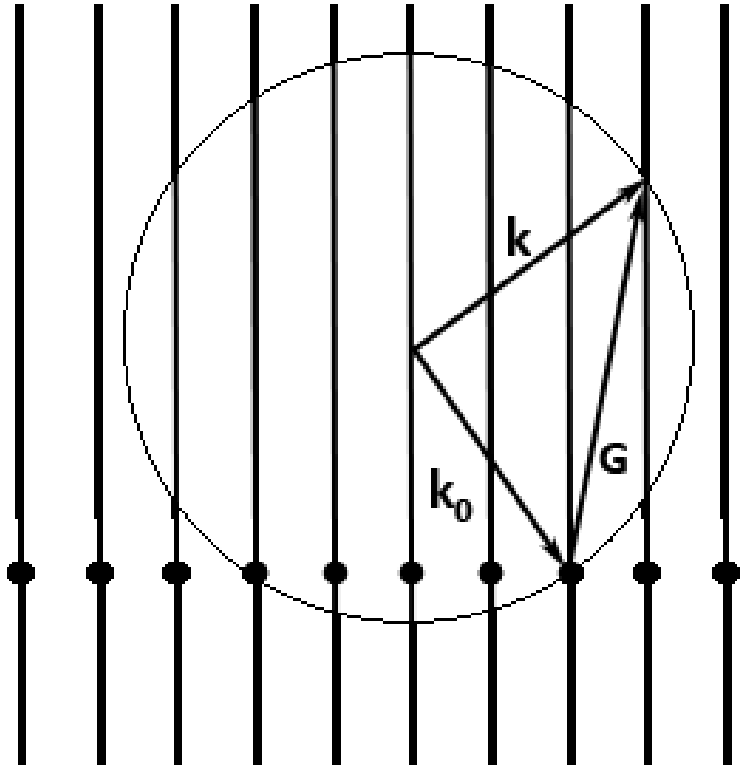




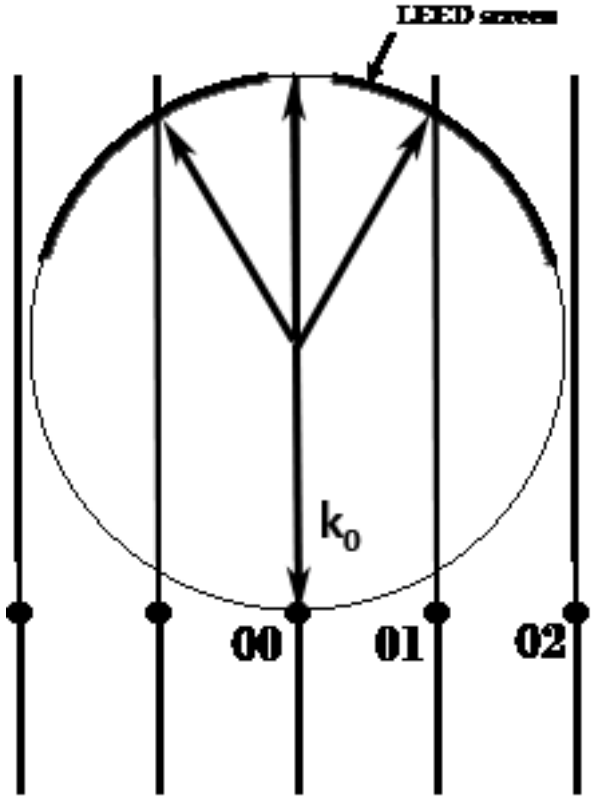
Low Energy Electron Difraction (LEED)



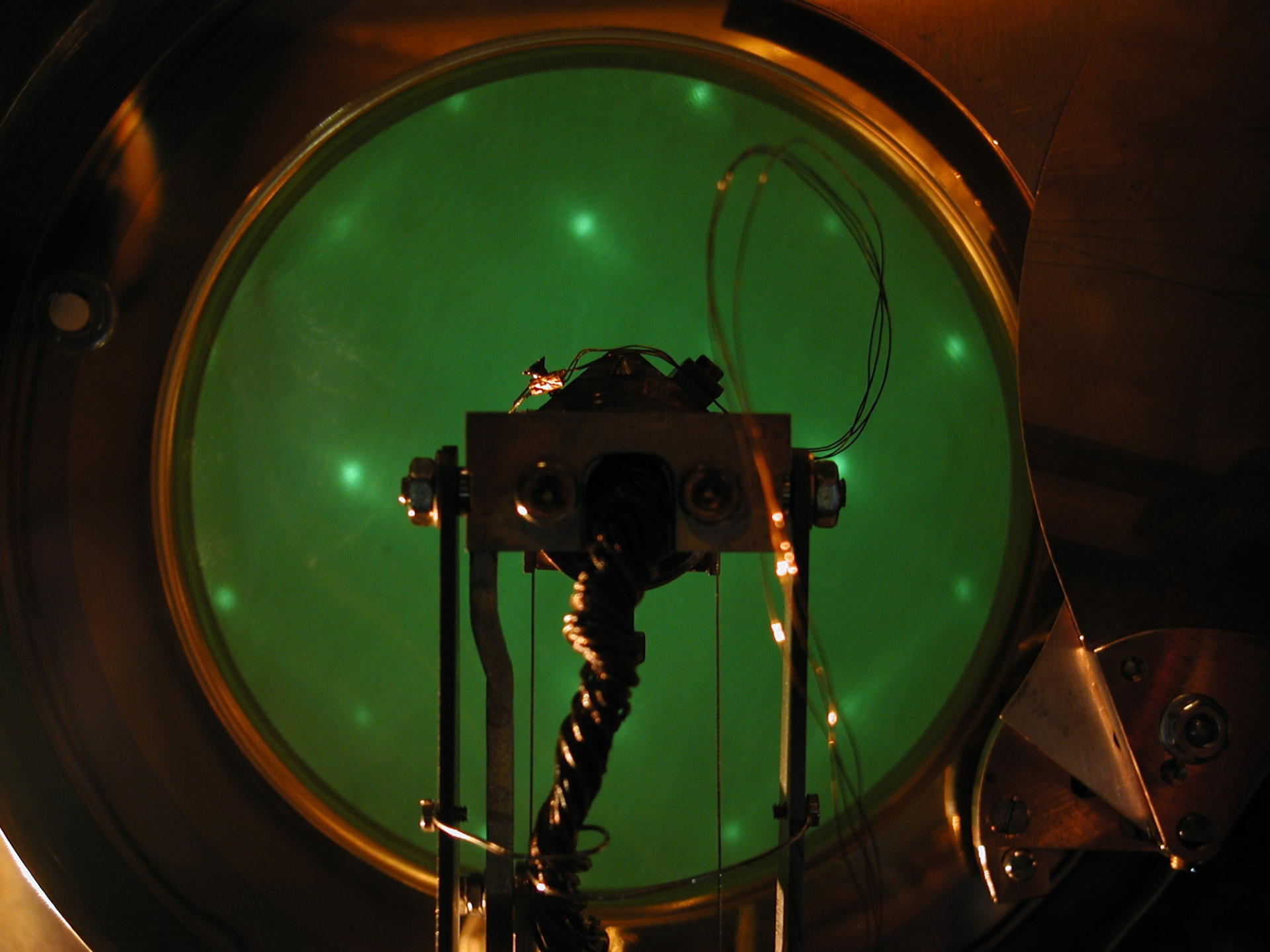

Real Space
LEED Pattern
a)
10
11
00
01
a
2π/a
b)
a
2π/a

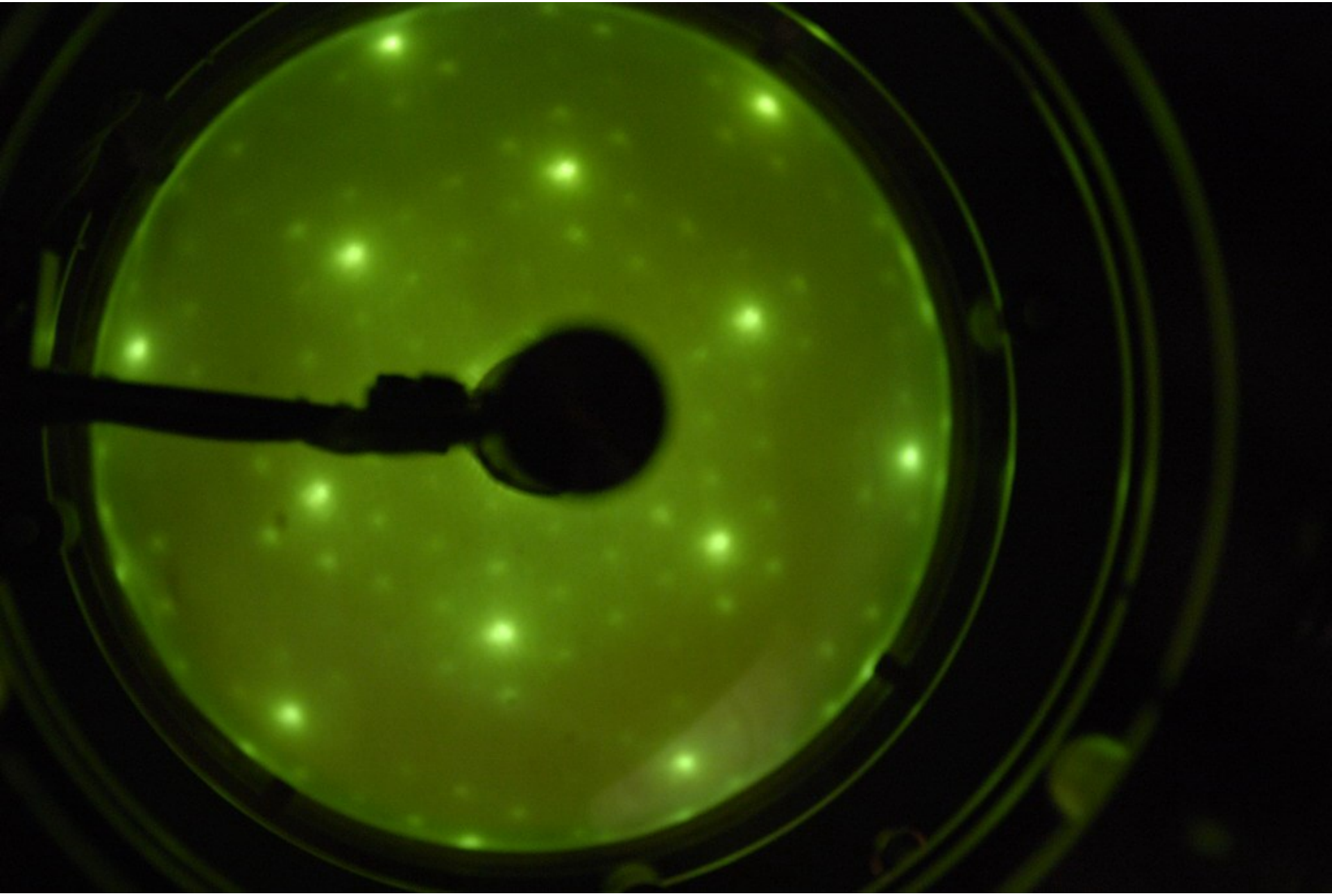


Ewald's sphere construction for the case of diffraction from a 2D-lattice. The intersections between Ewald's sphere and reciprocal lattice rods define the allowed diffracted beams.

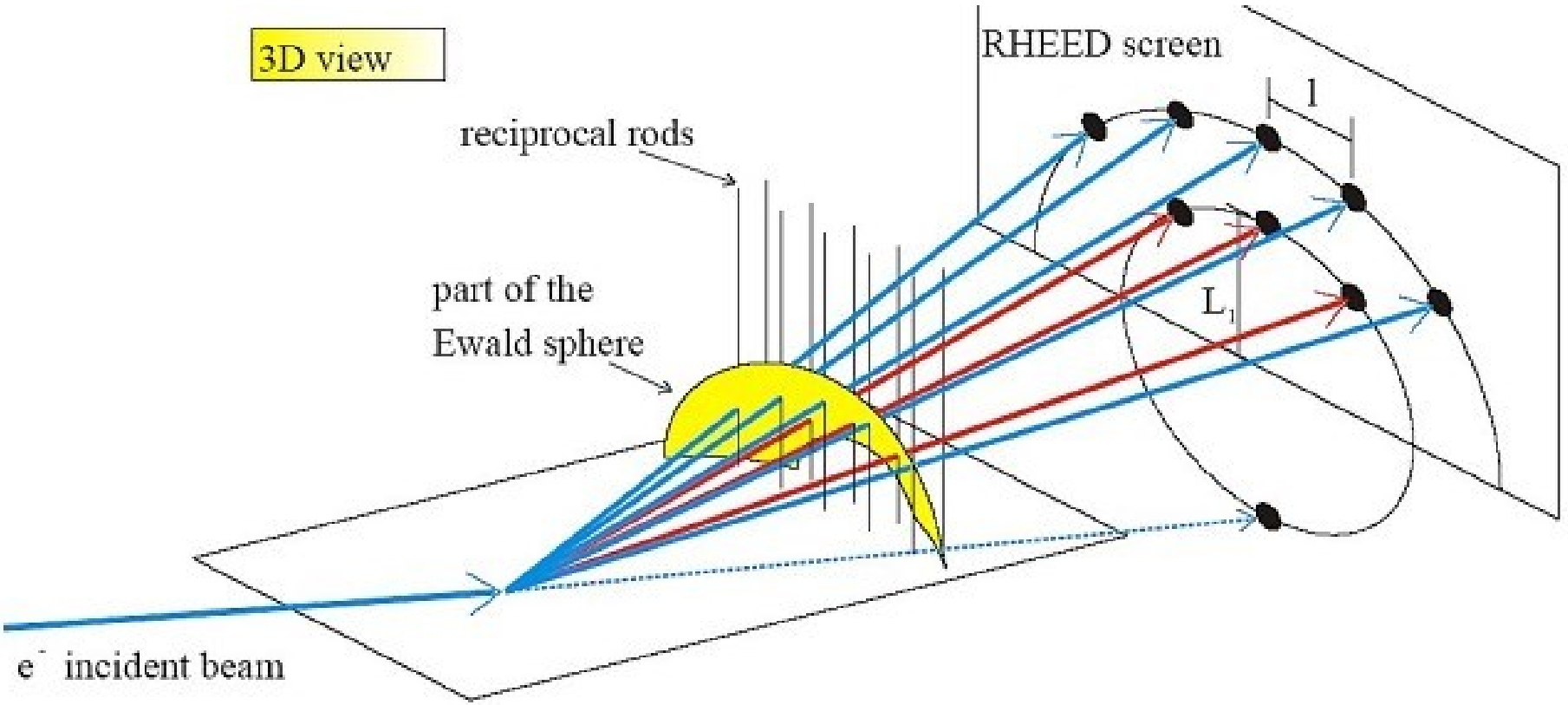


Ewald's sphere construction for the case of normal incidence of the primary electron beam. The diffracted beams are indexed according to the values of h and l.



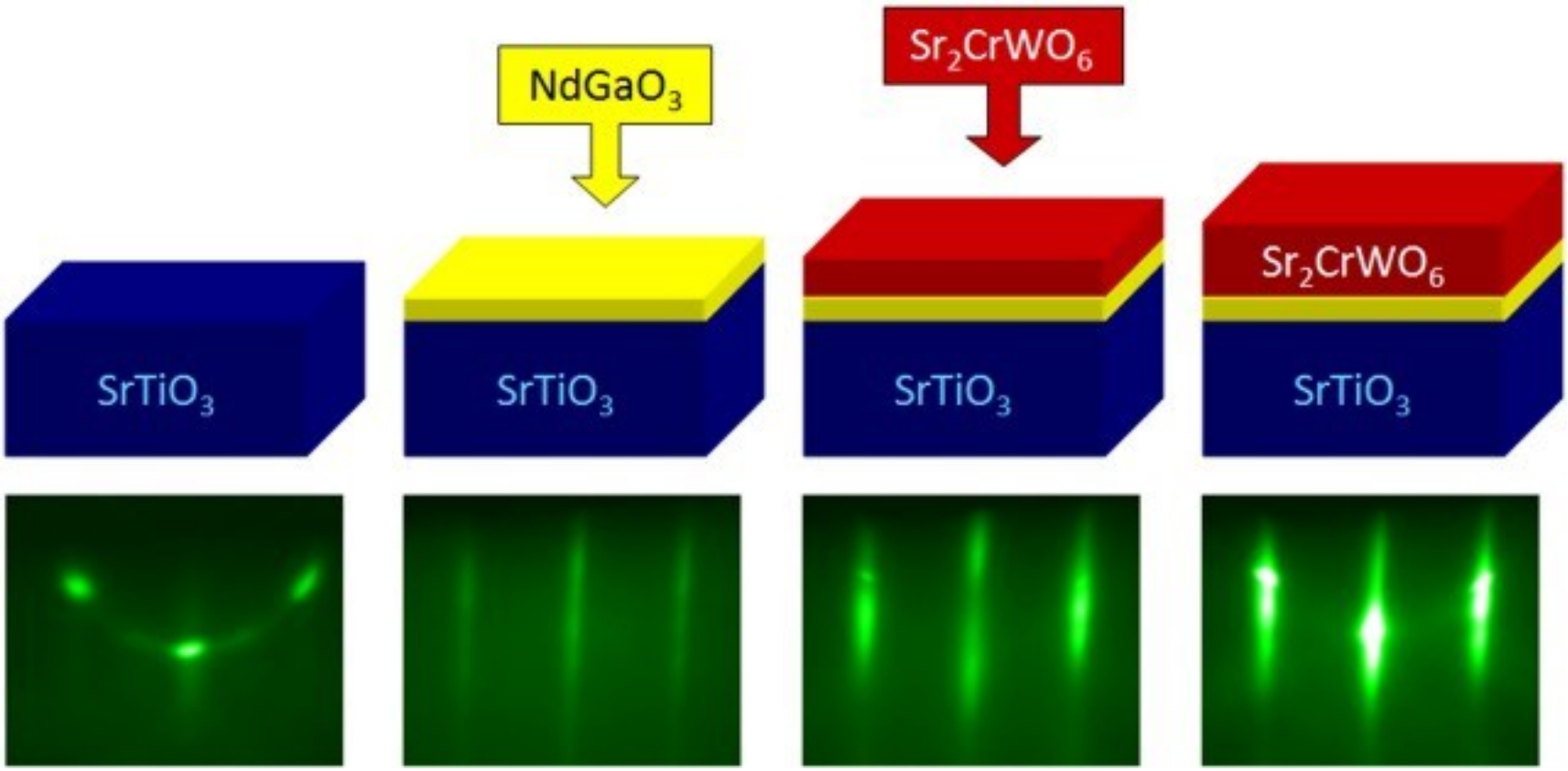


Reflection High Energy Electron Diffraction (**RHEED**)



Jürgen Klein, Epitaktische Heterostrukturen aus dotierten Manganaten,
PhD Thesis, University of Cologne (2001)
http://www.wmi.badw.de/methods/leed_rheed.htm

Reflection High Energy Electron Diffraction (**RHEED**)



Jürgen Klein, Epitaktische Heterostrukturen aus dotierten Manganaten,
PhD Thesis, University of Cologne (2001)
http://www.wmi.badw.de/methods/leed_rheed.htm

Reflection High Energy Electron Diffraction (**RHEED**)