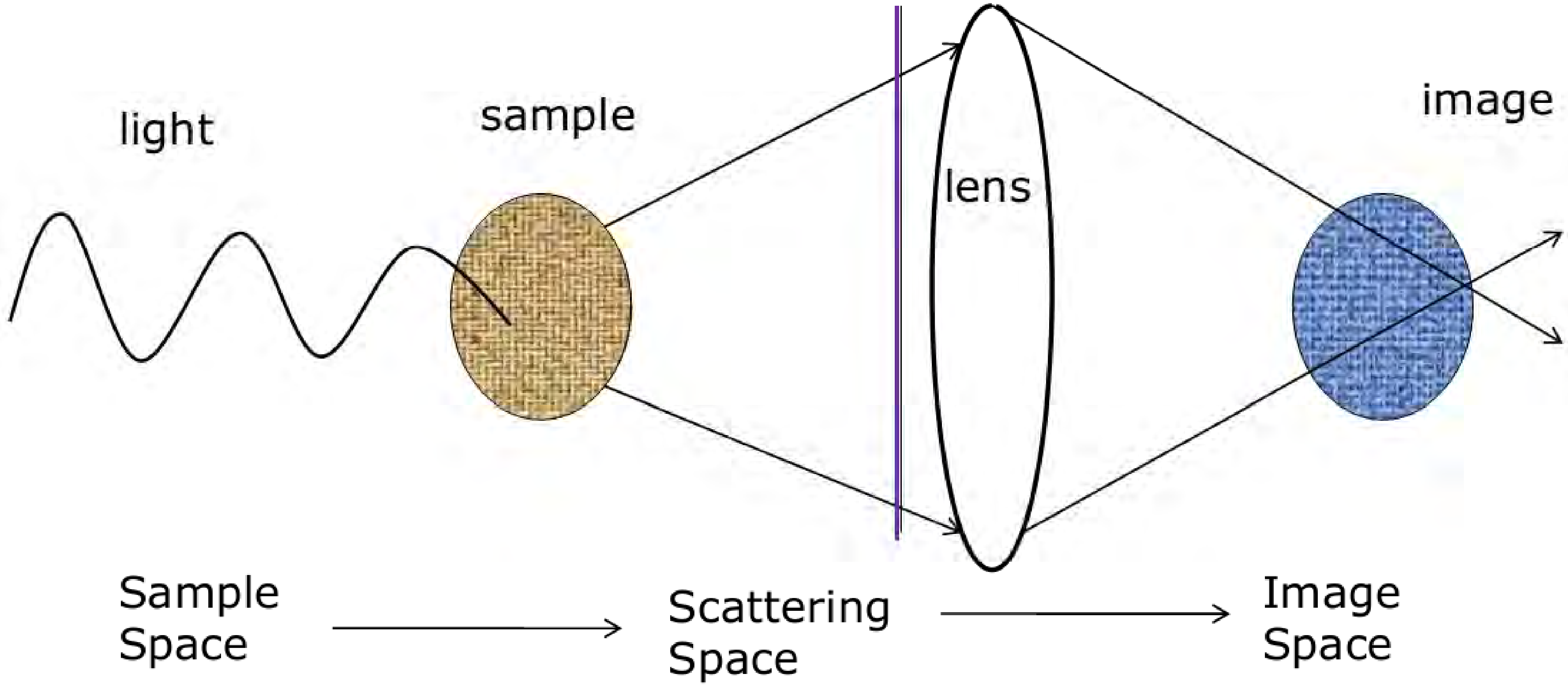
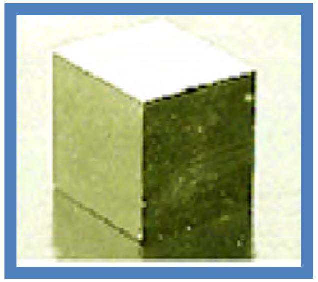
Jan-11-2013

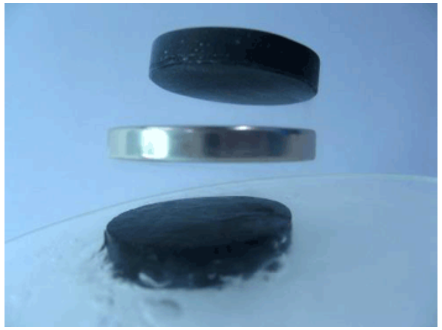
Thinking in Reciprocal space

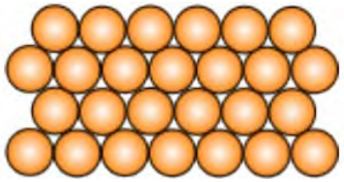


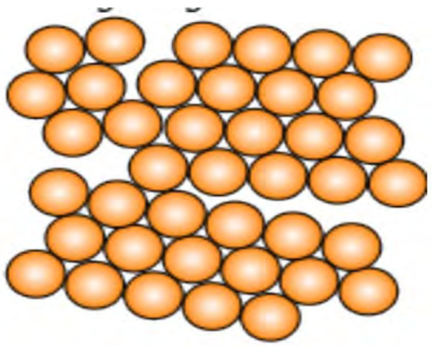
Acknowledge

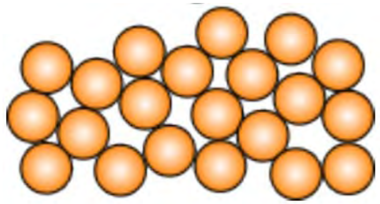
- Pengcheng's slides
- http://www.lks.physik.uni-erlangen.de/diffraction/space.htmlWikipedia
- http://www-ssrl.slac.stanford.edu/conferences/workshops/srxas-2012/documents/apurvamehta-srxas2012-thinkingreciprocalspace.pdf
- Others (google)



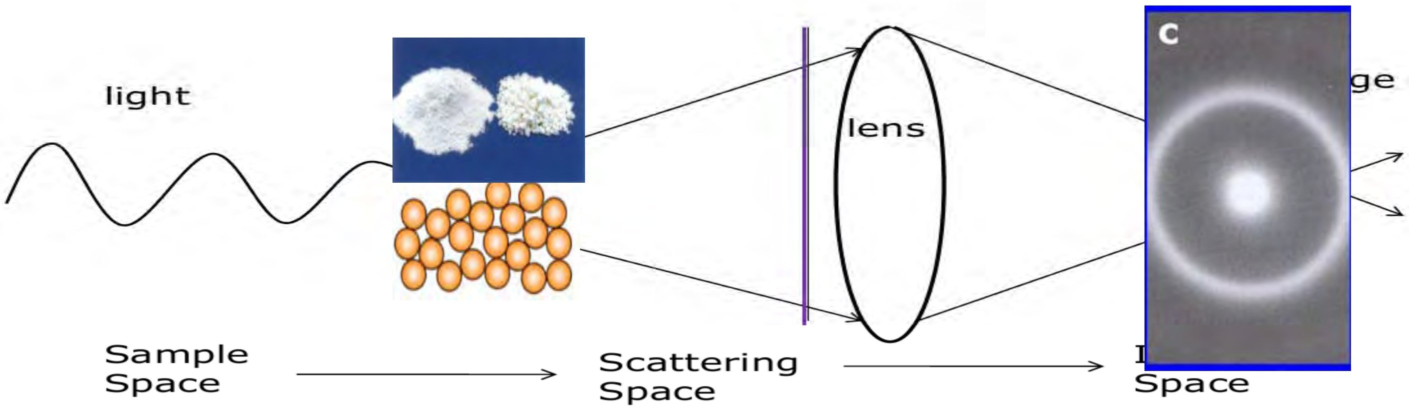








Amorporous


light
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c
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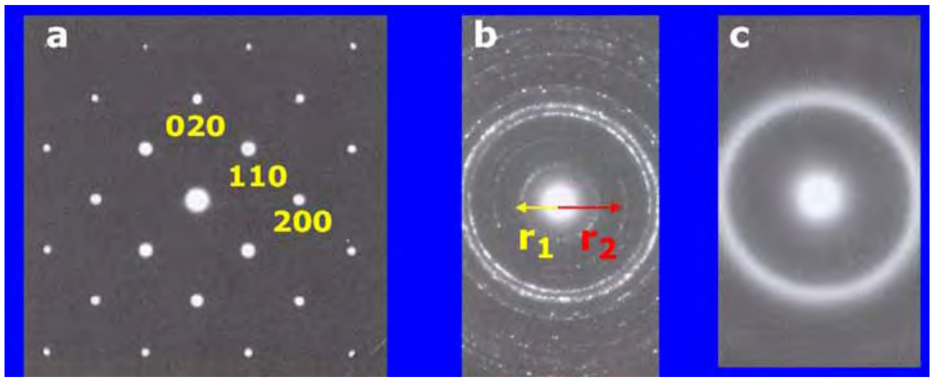
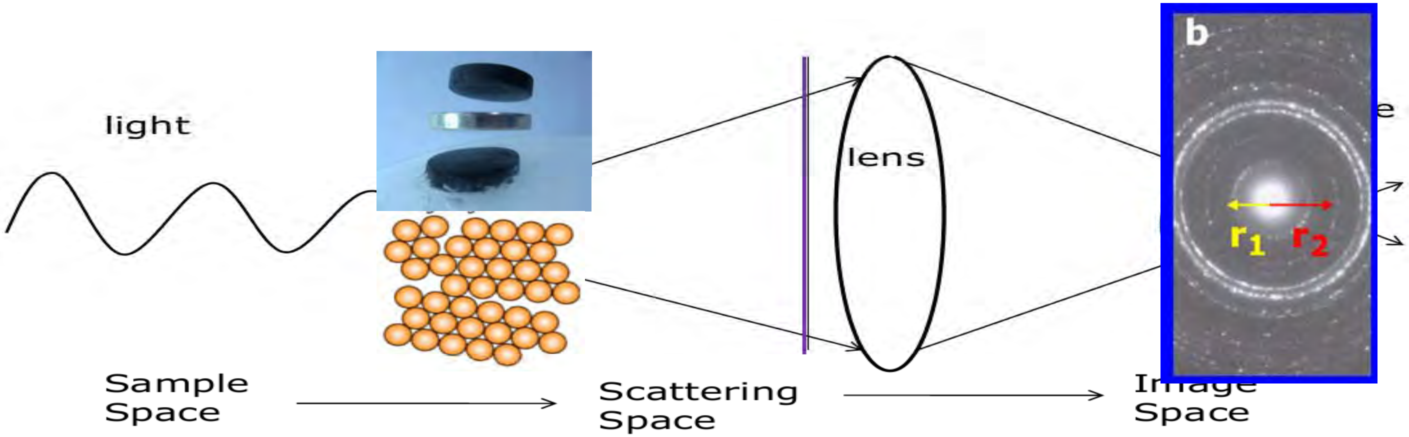
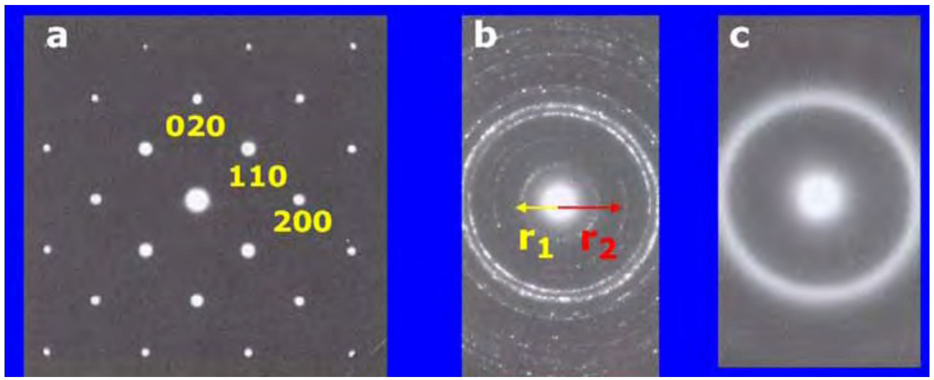
Sample
Space
Scattering
Space
I
Space

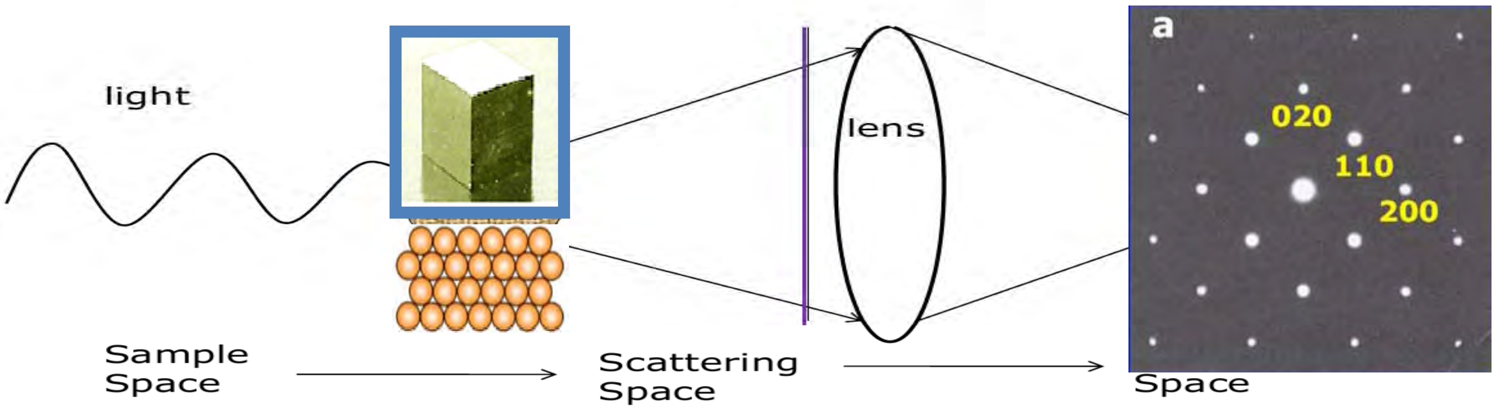

a
020
110
200
b
r1
r2
c

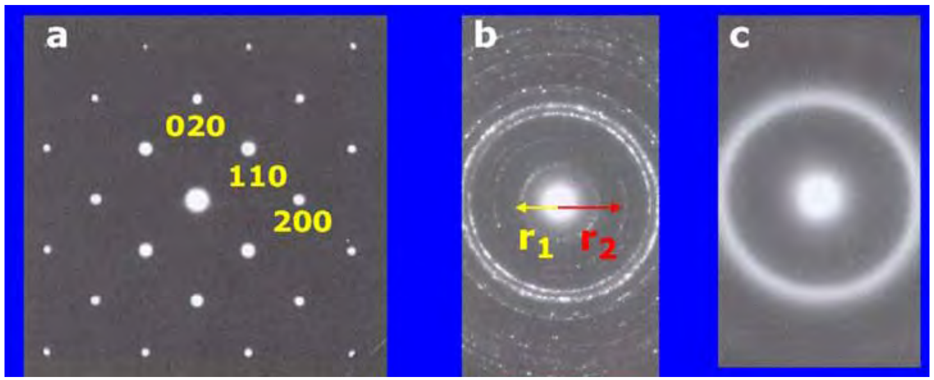
Polycrystal

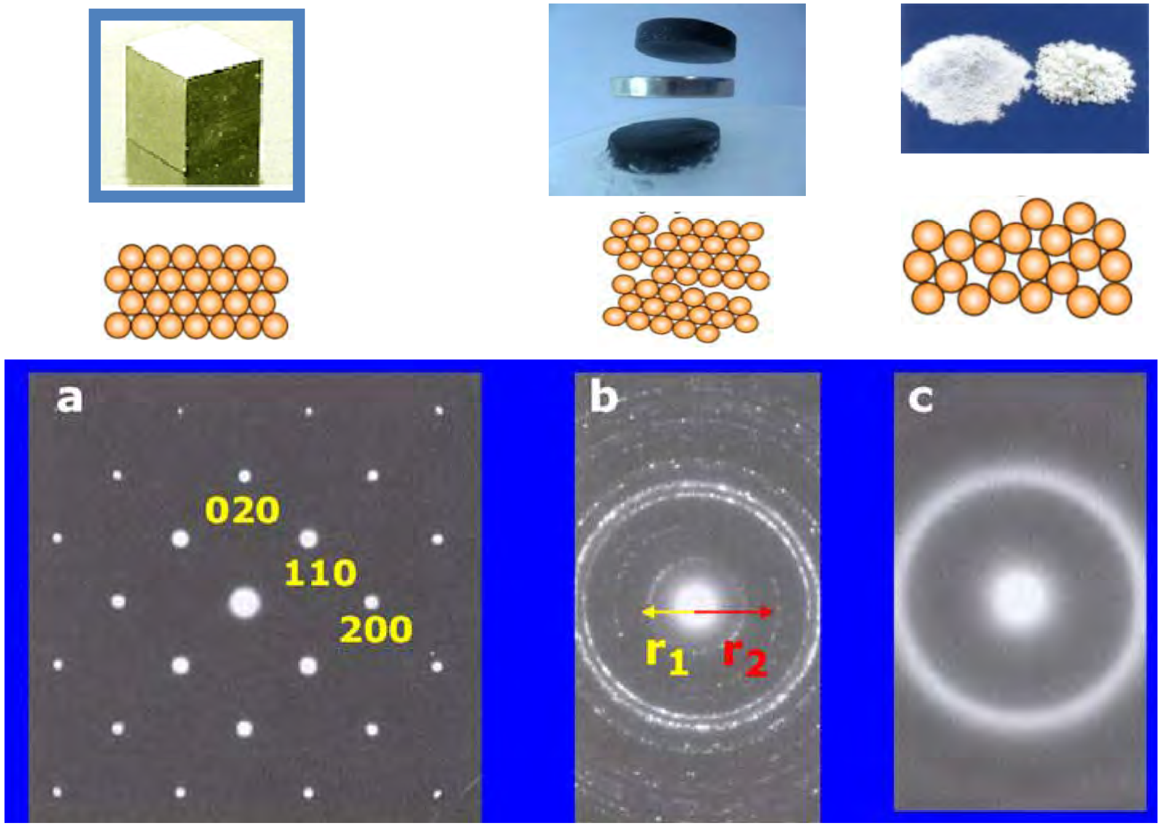




Single crystal






a
020
110
200
b
r1
r2
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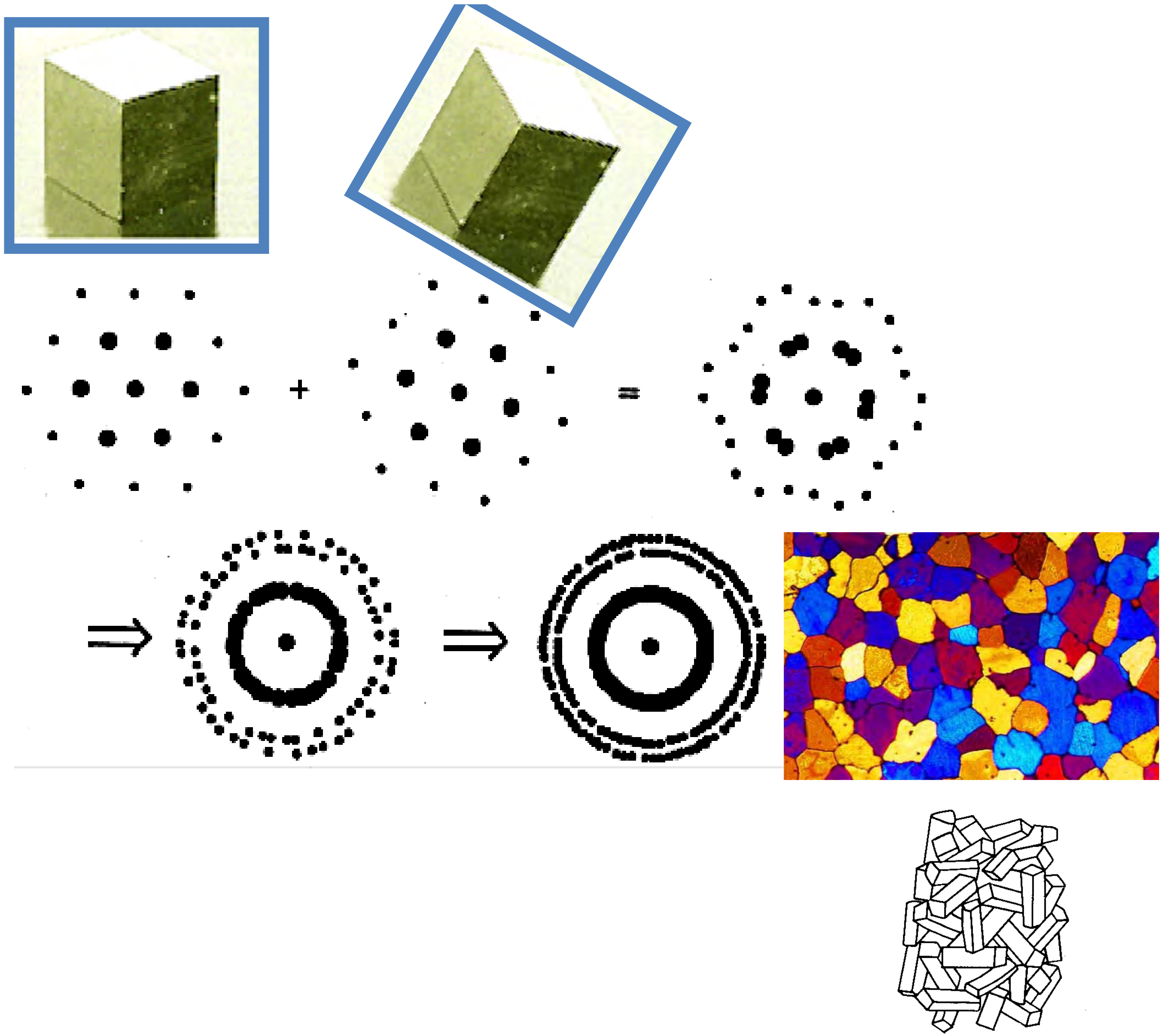
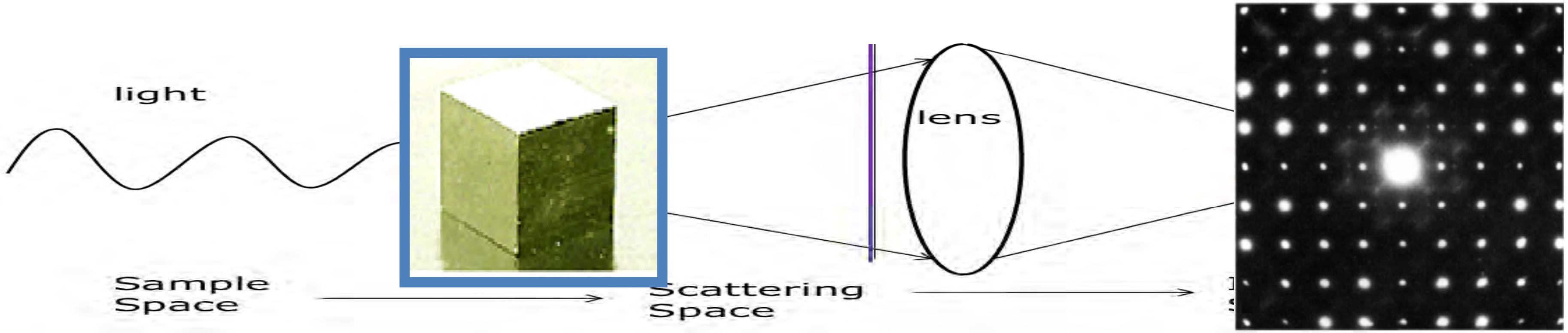


$$e^{i\mathbf{K}\cdot\mathbf{r}} = \cos(\mathbf{K}\cdot\mathbf{r}) + i\sin(\mathbf{K}\cdot\mathbf{r})$$

$$e^{i\mathbf{K}\cdot(\mathbf{r}+\mathbf{R})}$$



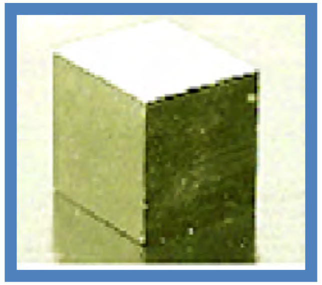
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

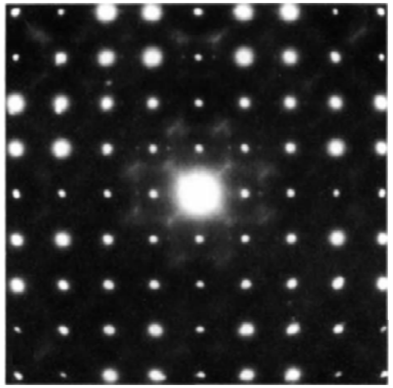
$$\mathbf{K} = k_1\mathbf{b_1} + k_2\mathbf{b_2} + k_3\mathbf{b_3}$$

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

$$\Rightarrow e^{i\mathbf{K}\cdot\mathbf{R}} = 1$$

$$\mathbf{K}\cdot\mathbf{R} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3)$$





$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$\mathbf{K} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$$

$$\mathbf{K}\cdot\mathbf{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

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

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

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

$$[\mathbf{b}_1\mathbf{b}_2\mathbf{b}_3]^T = 2\pi\,[\mathbf{a}_1\mathbf{a}_2\mathbf{a}_3]^{-1}.$$

The reciprocal of the reciprocal space is the real space. Examples of reciprocal lattice units.

Reciprocal lattice units in simple cubic case:

Let $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, and $\vec{a}_3 = a\hat{z}$

Prove that the reciprocal lattice primitive vectors satisfy

$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}.$$

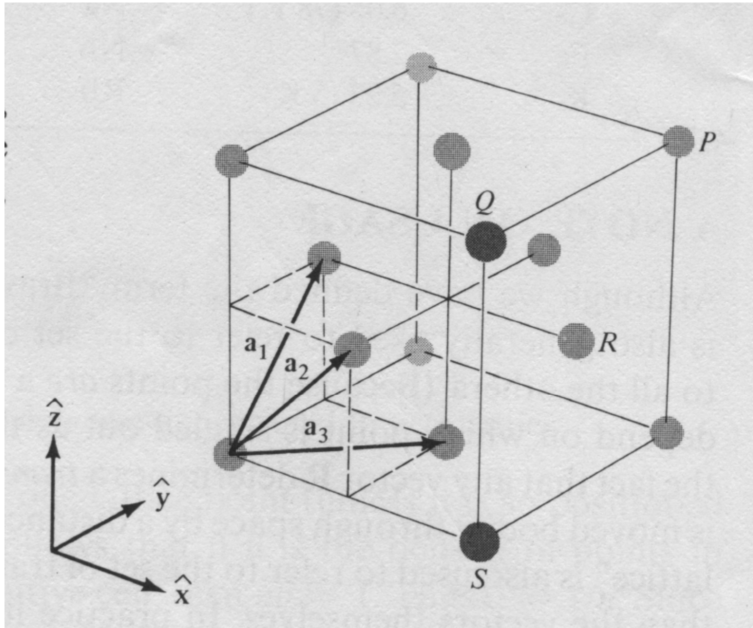
Note vector identity: $(\vec{c} \times \vec{a}) \times (\vec{a} \times \vec{b}) = (\vec{c} \cdot \vec{a} \times \vec{b})\vec{a}$

Reciprocal lattice units in fcc case:

Primitive vectors

$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}), \vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}), \vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}).$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}-\hat{x}), \vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x}-\hat{y}), \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}).$$

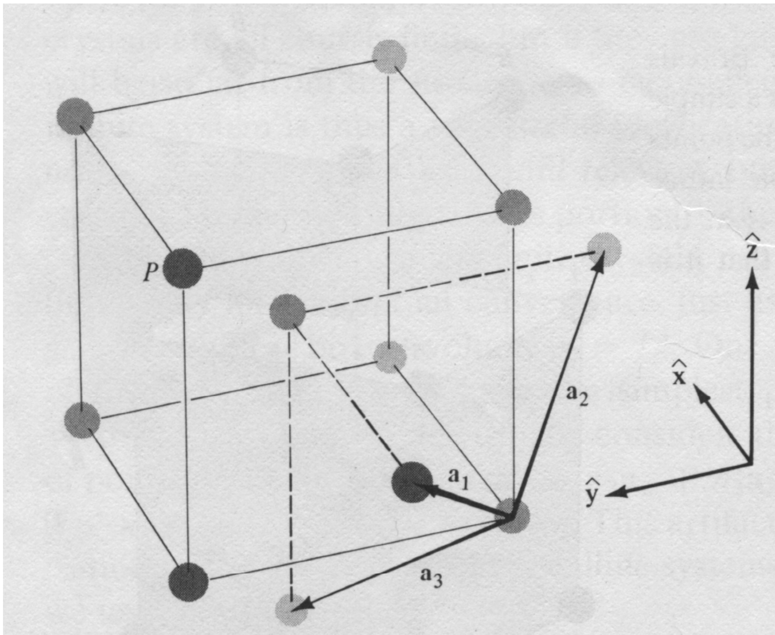


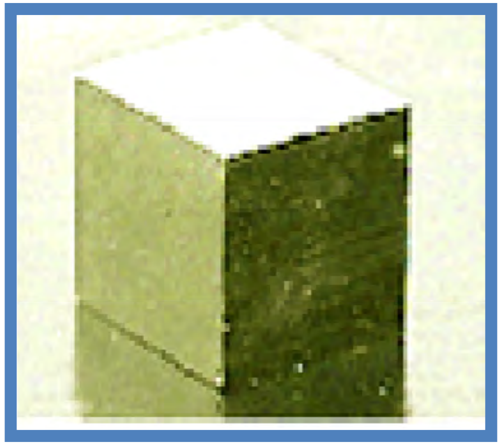
Reciprocal lattice units in bcc case:

Primitive vectors

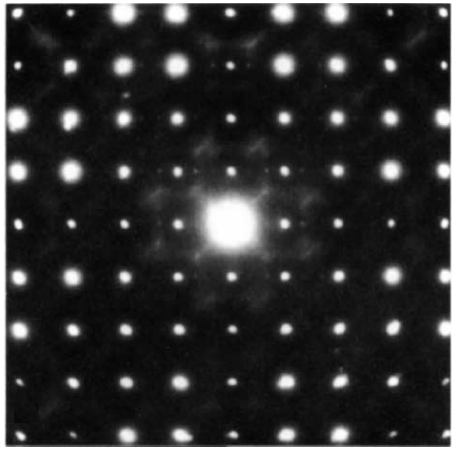
$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}-\hat{x}), \vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}-\hat{y}), \vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}).$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}), \vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x}), \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}).$$





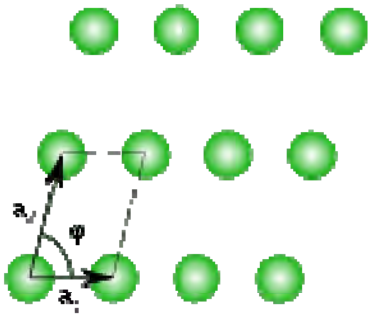
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$



$$\mathbf{K} = k_1\mathbf{b_1} + k_2\mathbf{b_2} + k_3\mathbf{b_3}$$

2D (5 lattice)

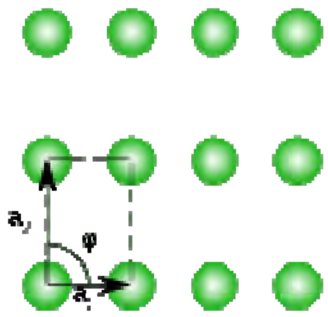
Parallelogram Lattice



$|a_1| \neq |a_2|, \varphi \neq 90°$

1

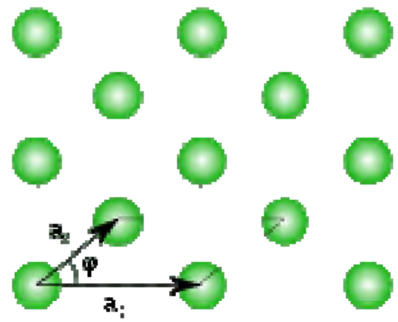
Rectangle Lattice



$|a_1| \neq |a_2|, \varphi = 90°$

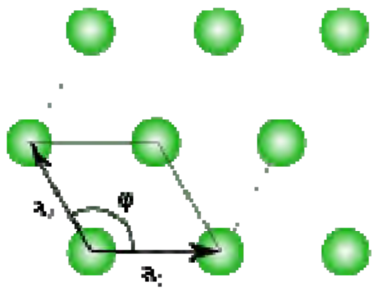
2

Centred Rectangle Lattice



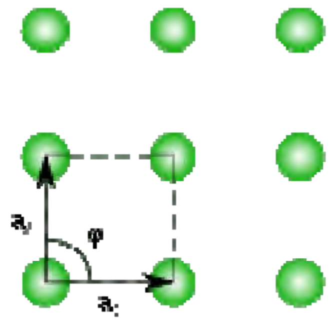
$|a_1| \neq |a_2|, \varphi \neq 90°$

3



$|a_1| = |a_2|, \varphi = 120°$

120° Rhombus Lattice



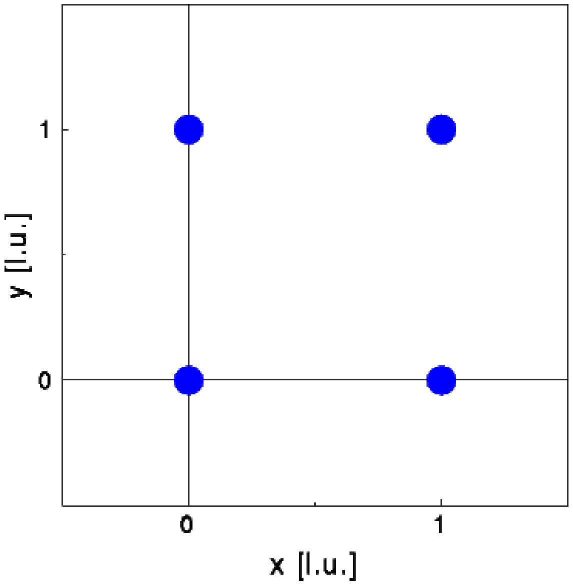
$|a_1| = |a_2|, \varphi = 90°$

5

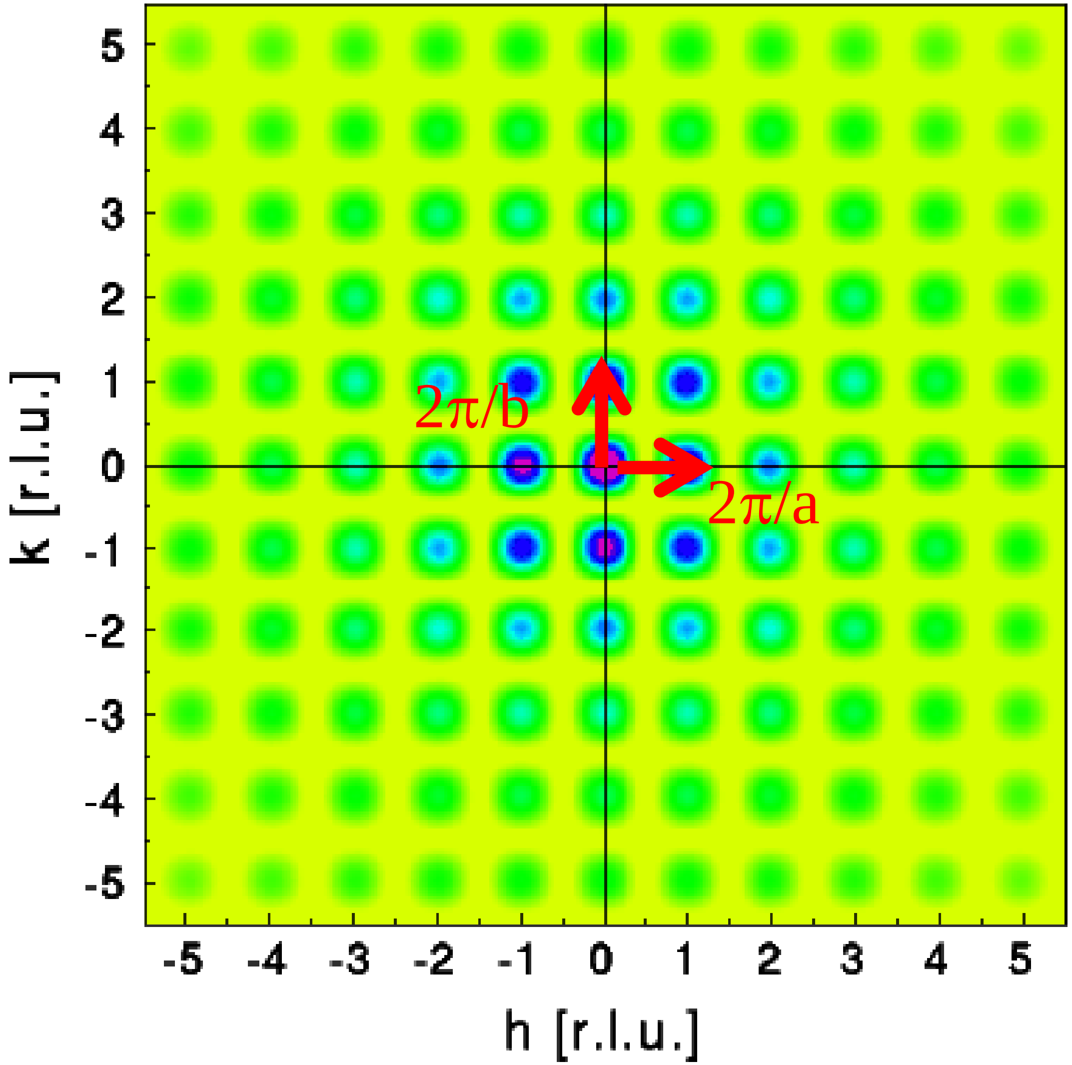
Square Lattice

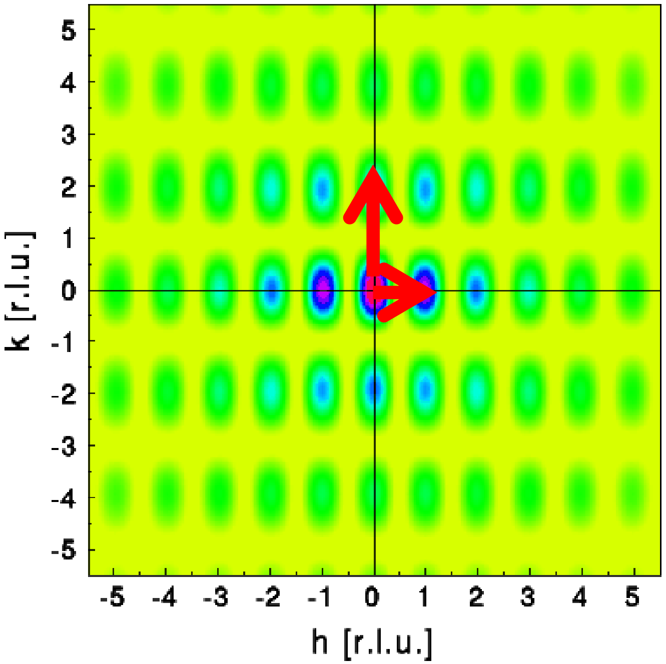
$$\mathbf{K}\cdot\mathbf{R} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3)$$

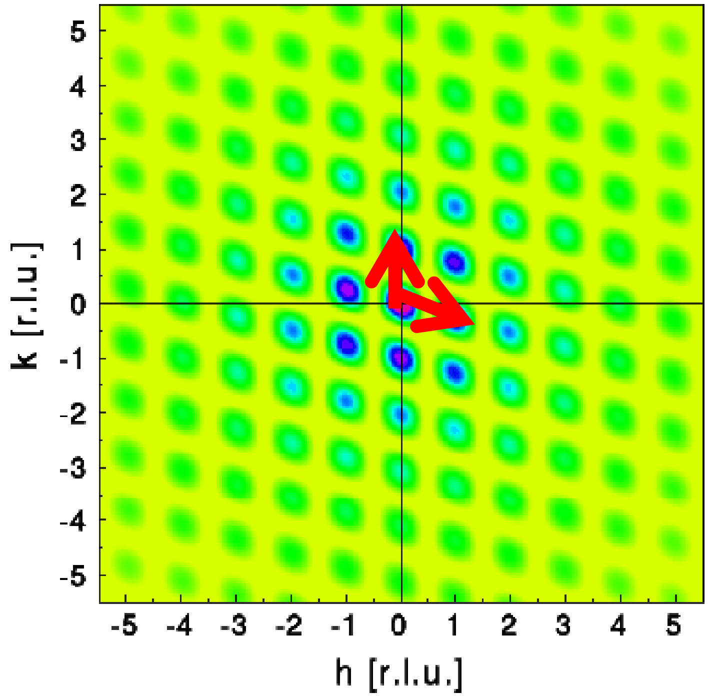
R space

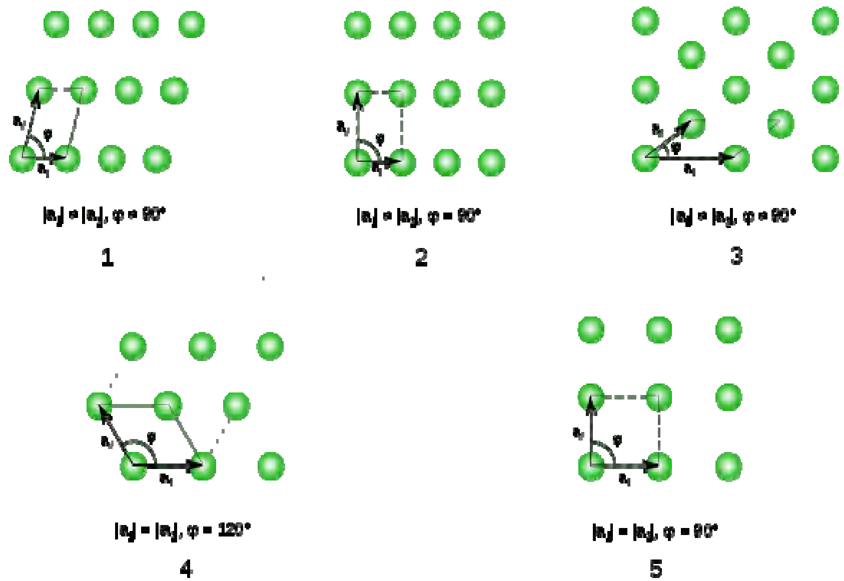


K space

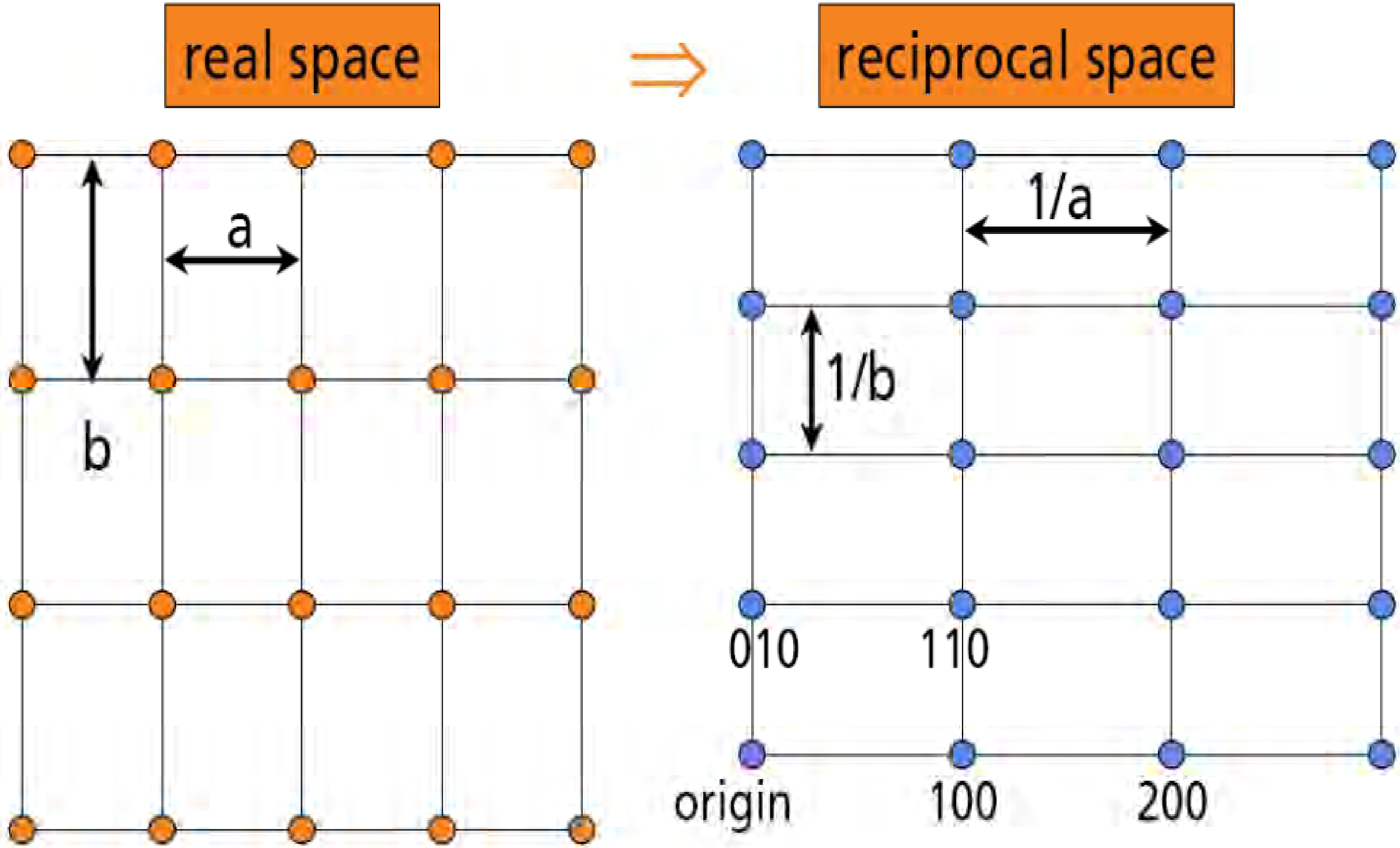



k [r.l.u.]
h [r.l.u.]
-5 -4 -3 -2 -1 0 1 2 3 4 5


k [r.l.u.]
h [r.l.u.]
-5 -4 -3 -2 -1 0 1 2 3 4 5


1
2
3
4
5

What is the Reciprocal Space? (1)

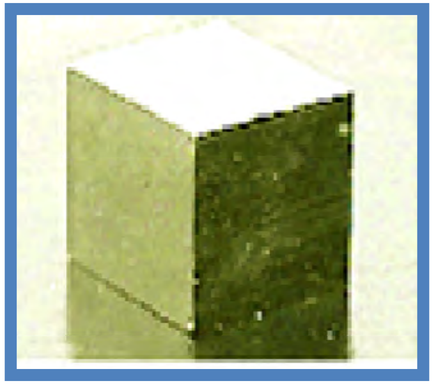


points represent atomic positions

points represent reflections

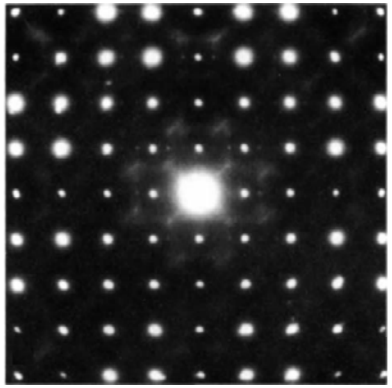
R space

K space

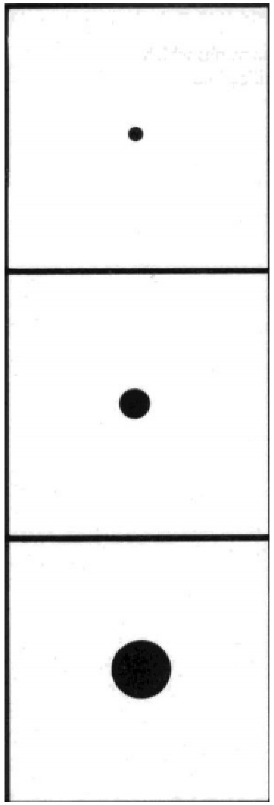


$$F(\vec{k}) = \int_{-\infty}^{\infty} f(\vec{r})e^{-i\vec{k}\cdot\vec{r}}d^3r.$$

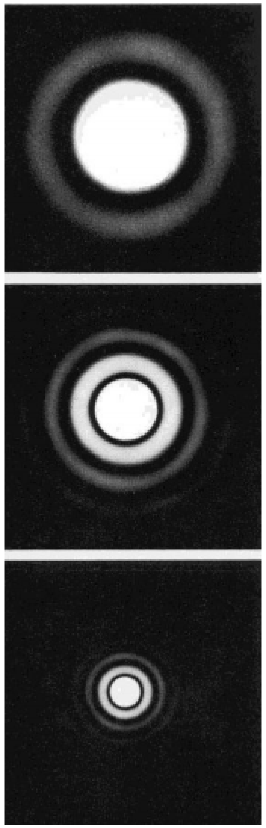
Fourier tranformation



$$\mathbf{K} \cdot \mathbf{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

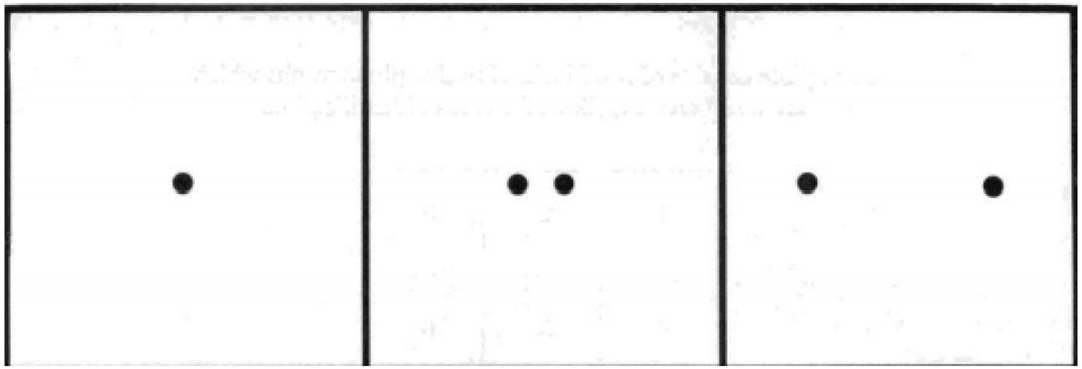


R space

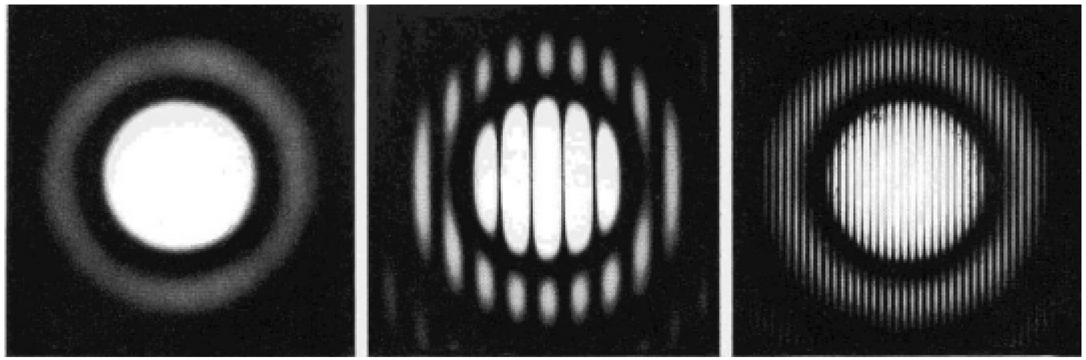


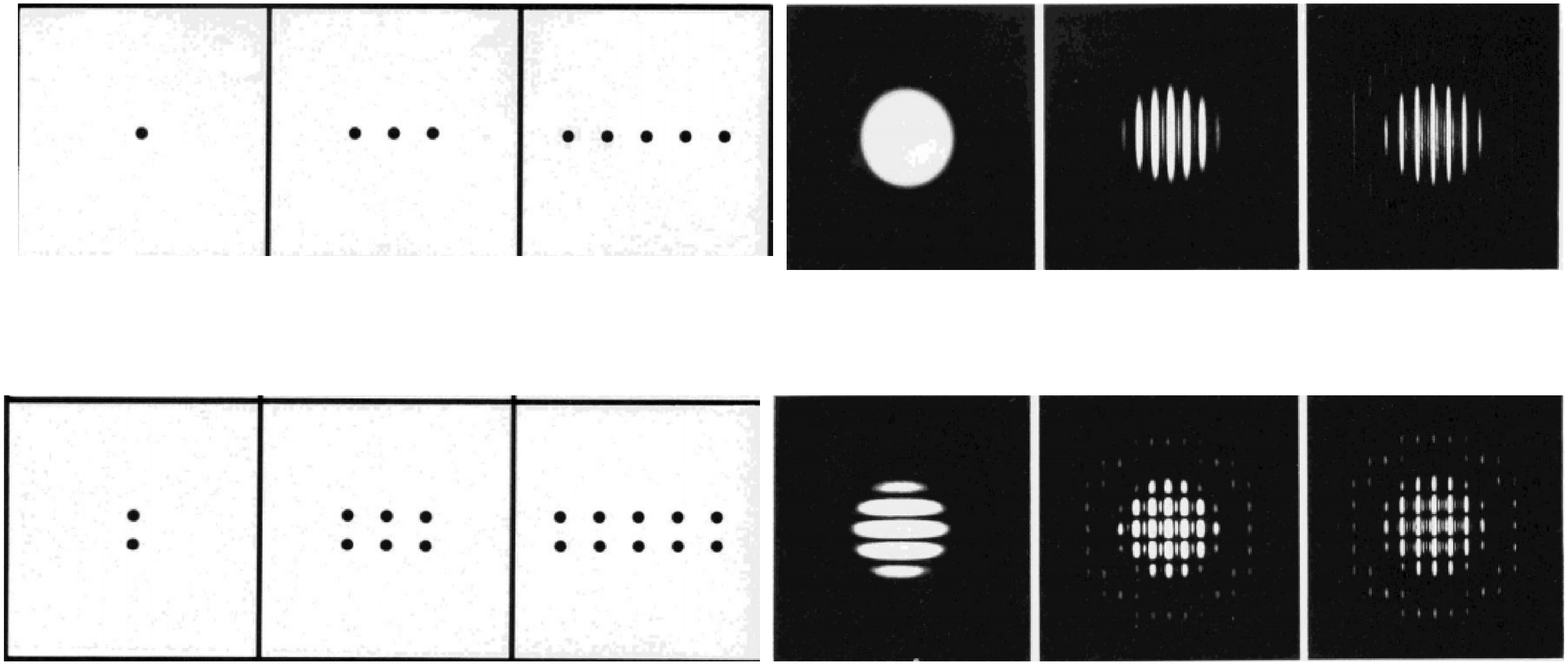
K space

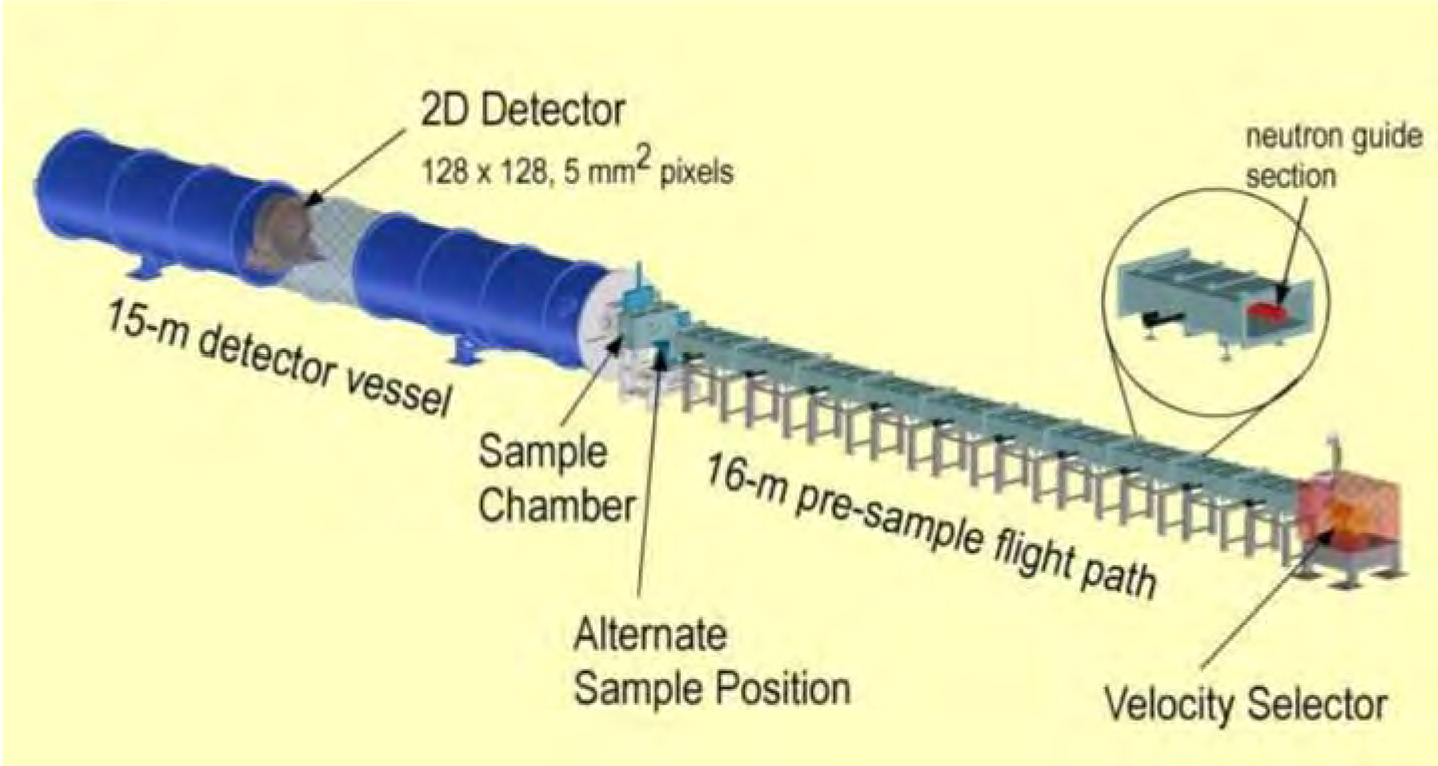
R space



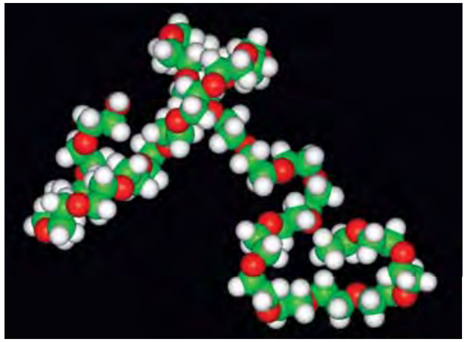
K space

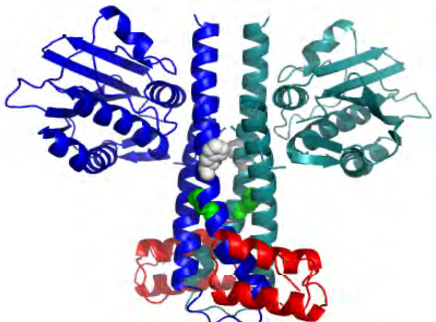


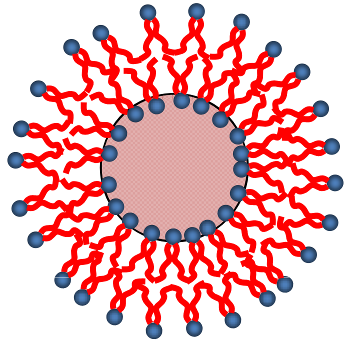


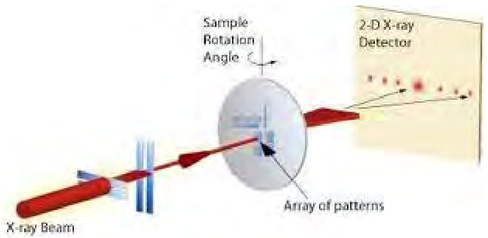


2D Detector
128 x 128, 5 mm2 pixels
neutron guide section
15-m detector vessel
Sample Chamber
16-m pre-sample flight path
Alternate Sample Position
Velocity Selector









Sample Rotation Angle
2-D X-ray Detector
X-ray Beam
Array of patterns