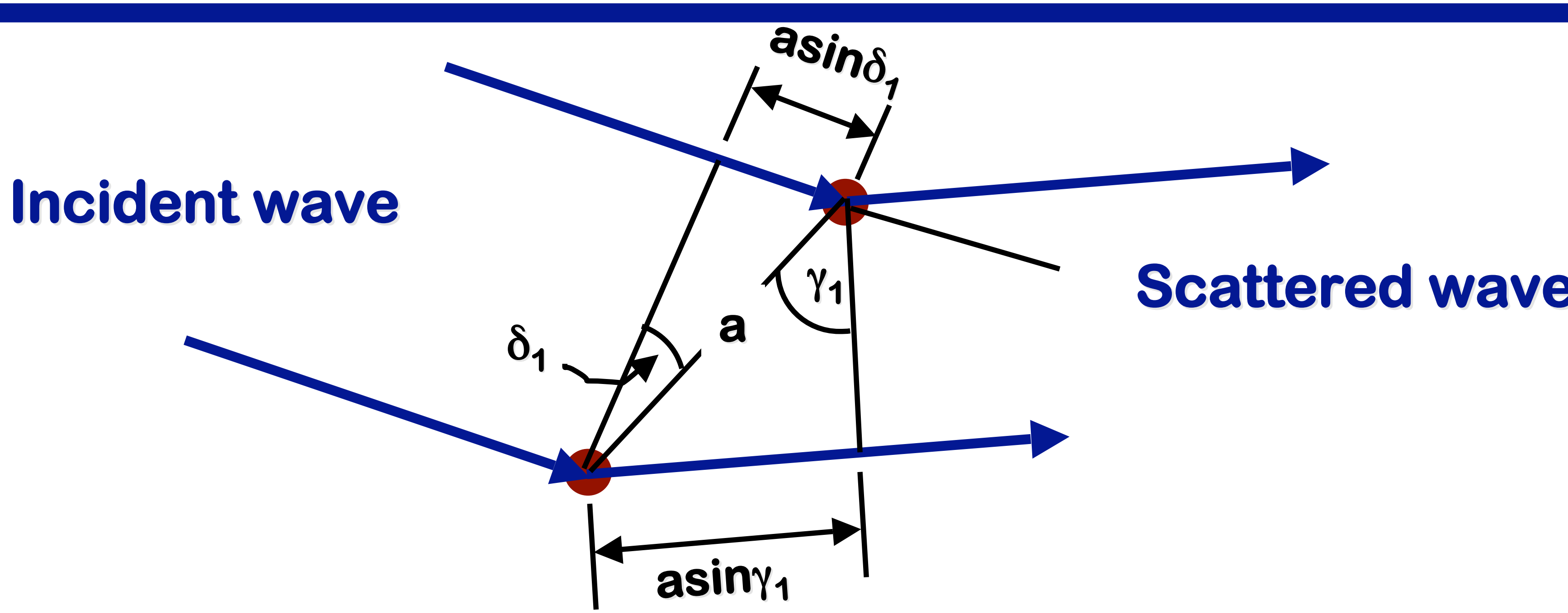
Laue diffraction and the reciprocal lattice

Lecture 4

Outline

- Laue Equations
- Reciprocal lattice
- Equivalence with Bragg's Law
- Ewald sphere construction
- Deviation parameter

Laue Equations



Constructive interference when:

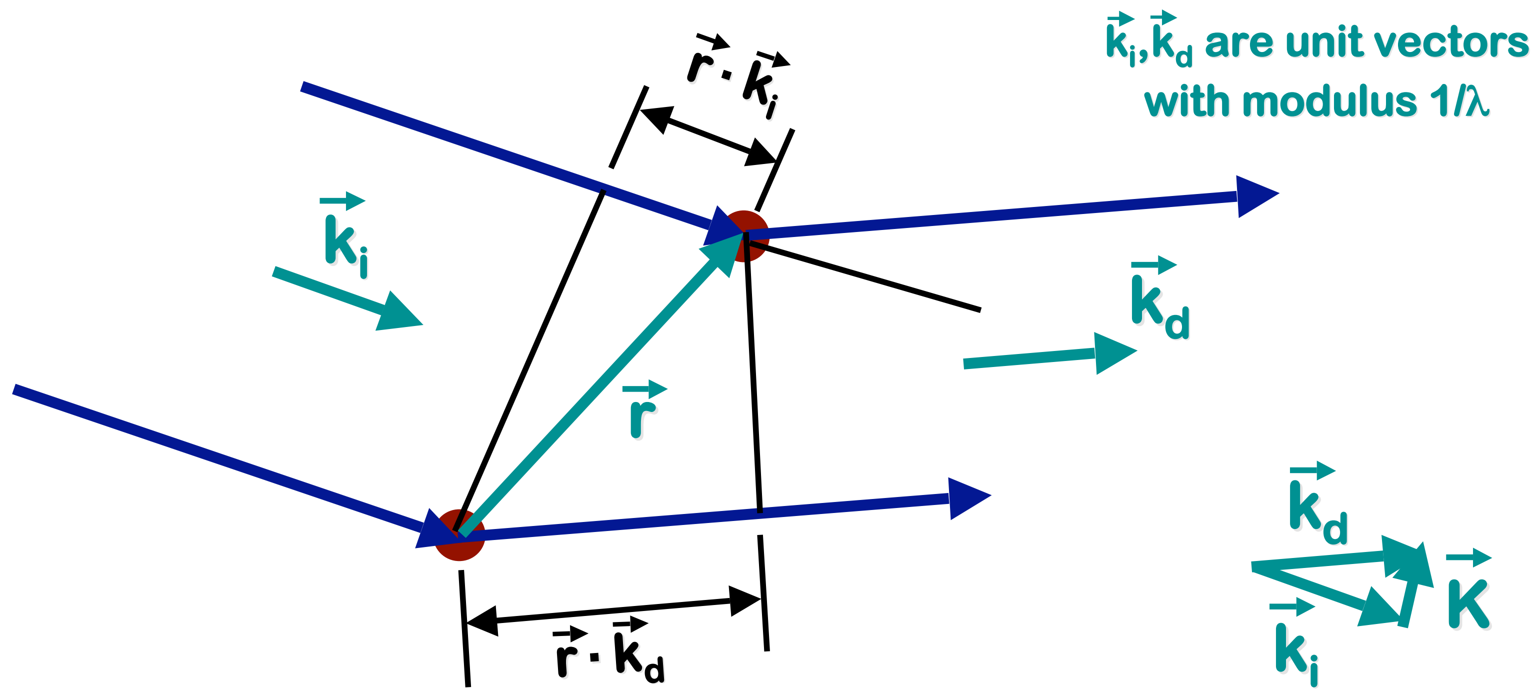
$$a(\sin\gamma_1 - \sin\delta_1) = h\lambda$$

$$b(\sin\gamma_2 - \sin\delta_2) = k\lambda$$

$$c(\sin\gamma_3 - \sin\delta_3) = l\lambda$$

h,k,l = integers

Laue Equations



$$\vec{r}\cdot\left(\vec{k}_d - \vec{k}_i\right) = \vec{r}\cdot\vec{K} = m \quad \text{with } m = \text{integer}$$

Resolve onto <u>lattice</u> unit vectors

$$\vec{K}\cdot\vec{a} = h$$

$$\vec{K}\cdot\vec{b} = k$$

$$\vec{K}\cdot\vec{c} = l$$

with h,k,l = integers

Laue Equations

Diffraction occurs when:

$$\vec{K}\cdot\vec{a} = h$$

$$\vec{K}\cdot\vec{b} = k \qquad \text{with } h,k,l = \text{integers}$$

$$\vec{K}\cdot\vec{c} = l$$

A general solution to these simultaneous equations is:

$$\vec{K} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* = \vec{g}$$

Where $\vec{a}^*, \vec{b}^*$ and $\vec{c}^*$ define a new set of lattice vectors, which are related to $\vec{a}$, $\vec{b}$ and $\vec{c}$ according to:

$$\vec{a}^*\cdot\vec{a} = 1 \qquad \vec{a}^*\cdot\vec{b} = 0 \qquad \vec{a}^*\cdot\vec{c} = 0$$

$$\vec{b}^*\cdot\vec{a} = 0 \qquad \vec{b}^*\cdot\vec{b} = 1 \qquad \vec{b}^*\cdot\vec{c} = 0$$

$$\vec{c}^*\cdot\vec{a} = 0 \qquad \vec{c}^*\cdot\vec{b} = 0 \qquad \vec{c}^*\cdot\vec{c} = 1$$

Reciprocal lattice

This new lattice is referred to as the reciprocal lattice.

In real space:

$$\vec{r}_n = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

In reciprocal space:

$$\vec{r}^* = m_1\vec{a}^* + m_2\vec{b}^* + m_3\vec{c}^*$$

Several properties of the reciprocal lattice include:

$$\vec{a}^* \perp \vec{b} \ \& \ \vec{c} \qquad \vec{a}^* = \vec{b} \times \vec{c} / V \qquad V = \vec{a} \cdot \vec{b} \times \vec{c}$$

$$\vec{b}^* \perp \vec{a} \ \& \ \vec{c} \qquad \vec{b}^* = \vec{a} \times \vec{c} / V$$

$$\vec{c}^* \perp \vec{a} \ \& \ \vec{b} \qquad \vec{c}^* = \vec{a} \times \vec{b} / V$$

(volume of unit cell of real lattice)

(recall not all real lattices have orthogonal lattice vectors)

Reciprocal lattice

Consider a reciprocal lattice vector g such that:

$$\vec{g} = h\vec{a}^* + kb^* + lc^*$$

where h,k and l are both integers, and are the Miller Indices of a plane in real space (h k l)

This vector g has two important properties (which we will prove):

$$\vec{g} \perp (hkl) \quad \text{and} \quad |\vec{g}| = \frac{1}{d_{hkl}}$$

Reciprocal lattice

proofs

Prove: $\vec{g} \perp (hkl)$

1.) $\frac{\vec{a}}{h} + \overrightarrow{AB} = \frac{\vec{b}}{k}$

$\overrightarrow{AB} = \frac{\vec{b}}{k} - \frac{\vec{a}}{h}$

2.) Is $\vec{g} \perp \overrightarrow{AB}$?

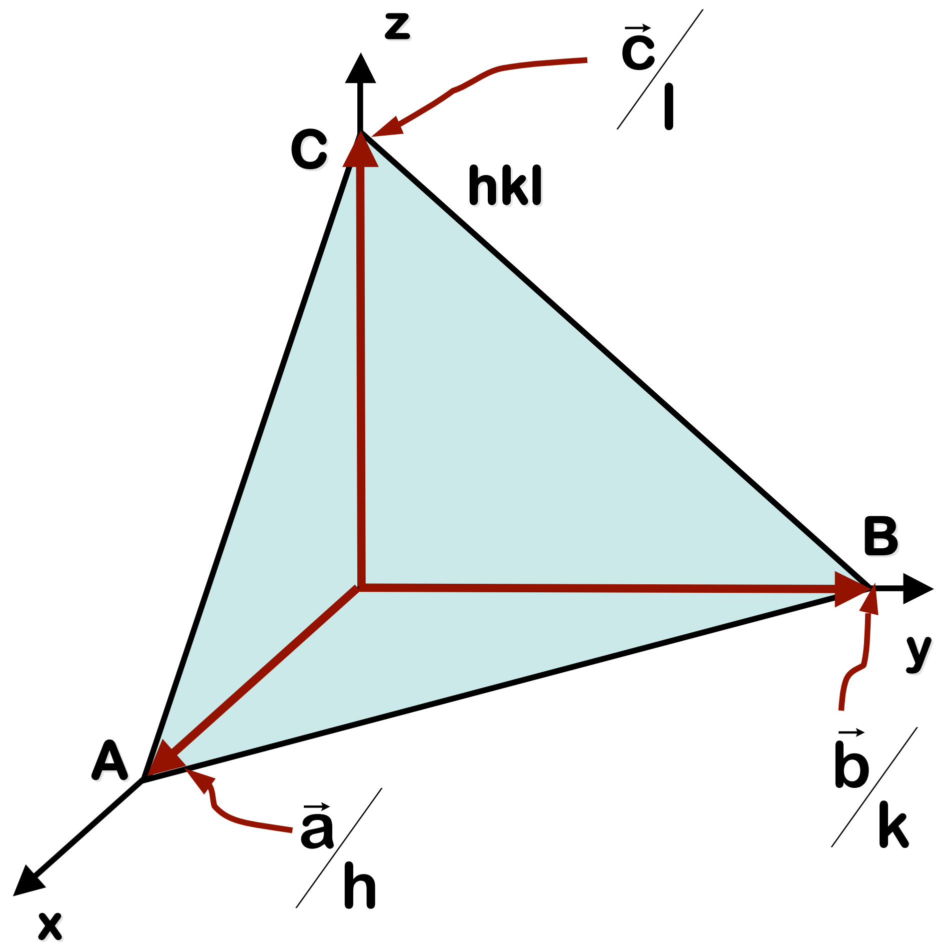
$\vec{g} \cdot \overrightarrow{AB} = 0$

$(ha^* + kb^* + lc^*) \cdot \left(\frac{\vec{b}}{k} - \frac{\vec{a}}{h}\right) = 0$

3.) Can repeat to show:

$\vec{g} \perp \overrightarrow{AC}$

4.) $\vec{g} \perp (hkl)$



$\vec{a}^* \cdot \vec{b} = \vec{a}^* \cdot \vec{c} = \vec{b}^* \cdot \vec{c} = \vec{b}^* \cdot \vec{a} = \vec{c}^* \cdot \vec{a} = \vec{c} \cdot \vec{b} = 0$

$\vec{a}^* \cdot \vec{a} = \vec{b}^* \cdot \vec{b} = \vec{c}^* \cdot \vec{c} = 1$

Reciprocal lattice

proofs

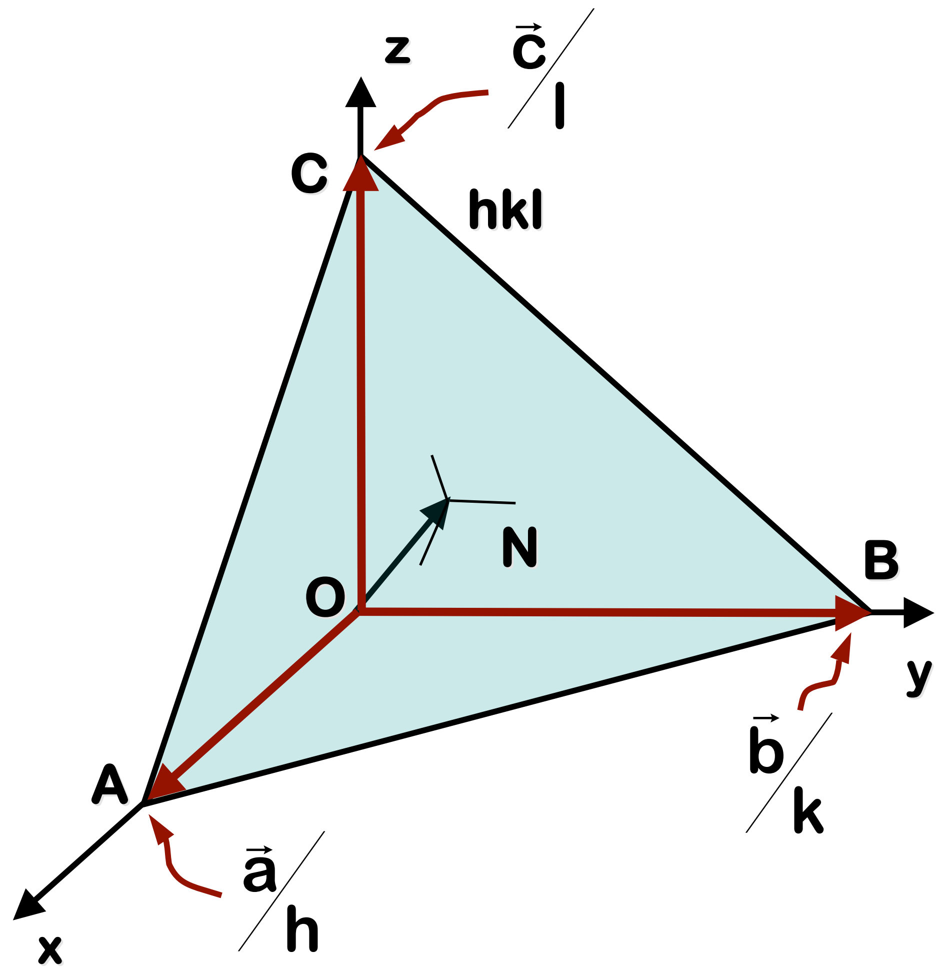
Prove: $|\vec{g}| = \frac{1}{d_{hkl}}$

Shortest distance must be projection of real lattice vector on to a unit vector in direction $\vec{g}$ (define as $\vec{n}$)

$$d_{hkl} = ON = \frac{\vec{a}}{h} \cdot \vec{n} = \frac{\vec{a}}{h} \cdot \frac{\vec{g}}{|\vec{g}|}$$

$$d_{hkl} = \frac{\vec{a}}{h} \cdot \frac{h\vec{a}^* + k\vec{b}^* + l\vec{c}^*}{|\vec{g}|} = \frac{1}{|\vec{g}|}$$

$$|\vec{g}| = \frac{1}{d_{hkl}}$$

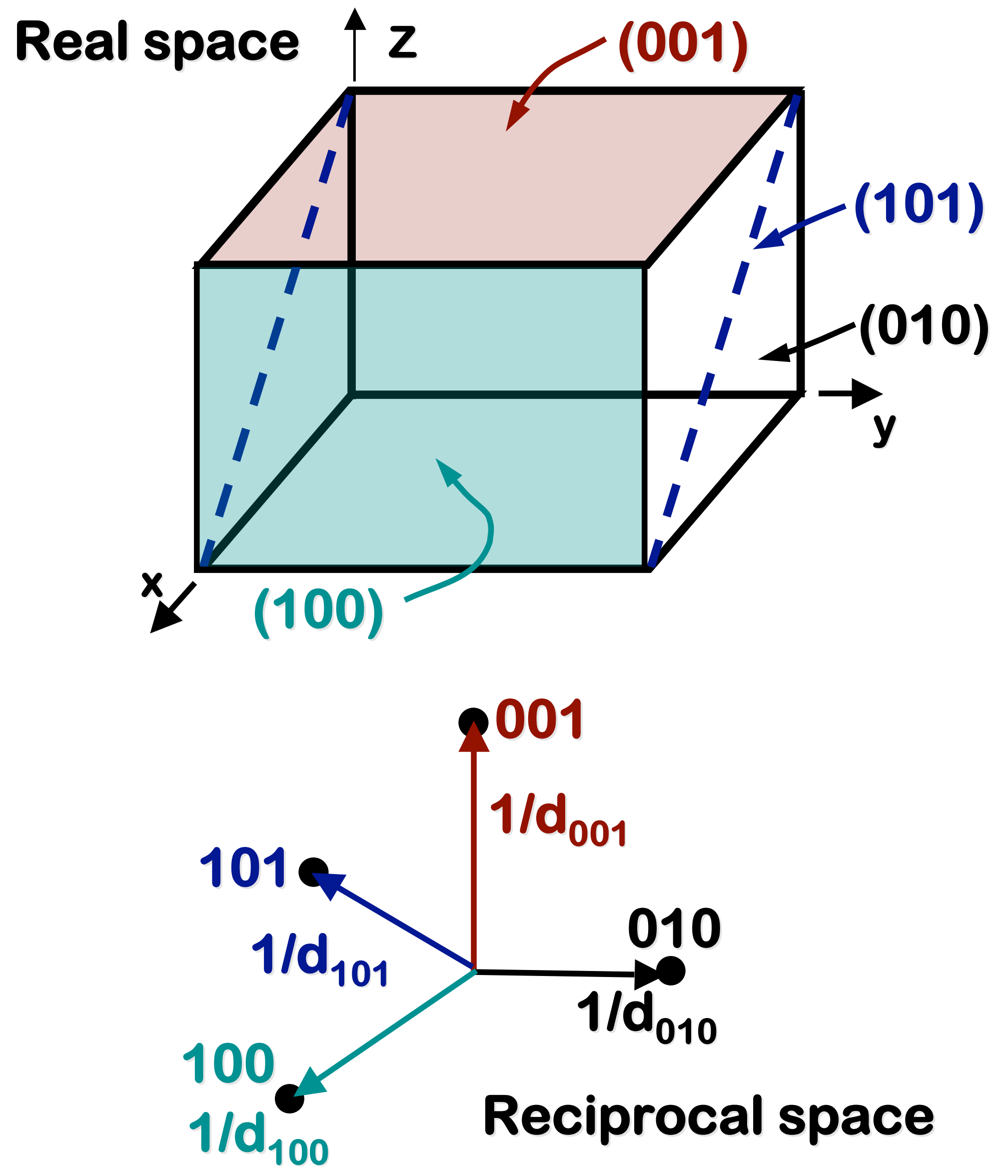


Reciprocal lattice

Reciprocal lattice *points* each correspond to a *plane* in real space

Reciprocal lattice points are defined by reciprocal lattice vectors where:

$$\vec{g} \perp (hkl) \quad \text{and} \quad d_{hkl} = \frac{1}{|\vec{g}|}$$



Real => Reciprocal

The relationship between real and reciprocal determined by:

$$\vec{a}^* \cdot \vec{a} = 1 \quad \vec{a}^* \cdot \vec{b} = 0 \quad \vec{a}^* \cdot \vec{c} = 0$$

$$\vec{b}^* \cdot \vec{a} = 0 \quad \vec{b}^* \cdot \vec{b} = 1 \quad \vec{b}^* \cdot \vec{c} = 0$$

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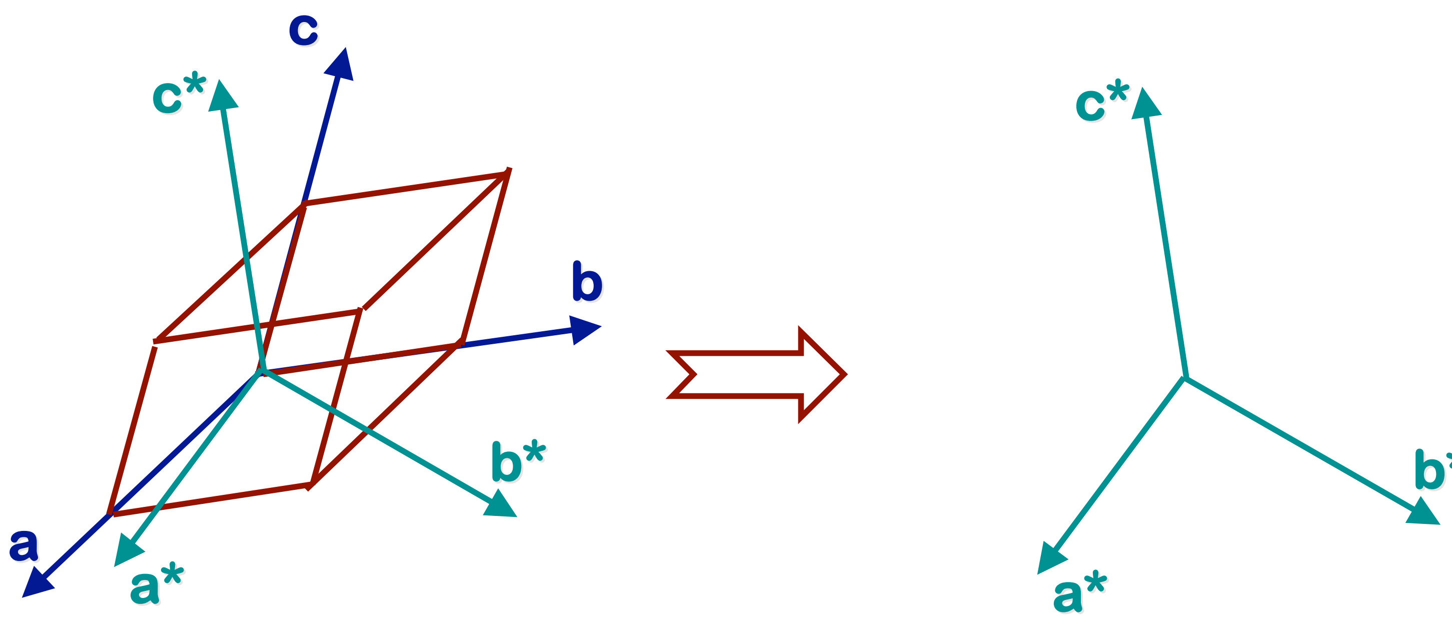
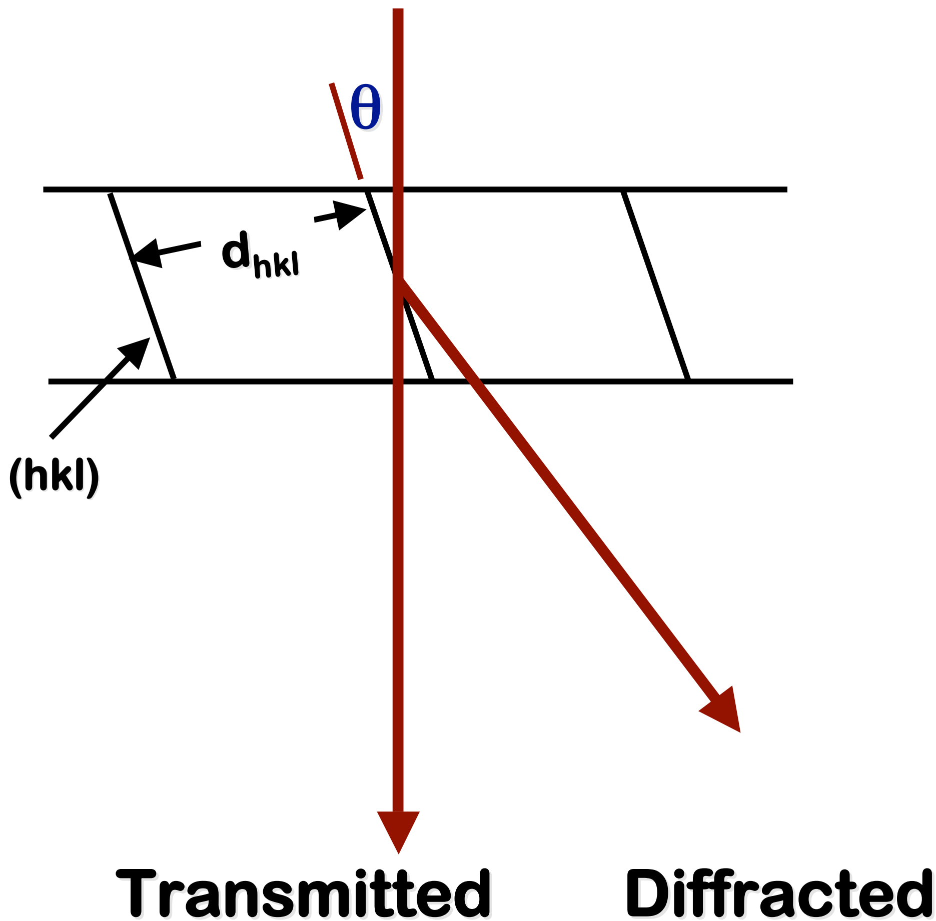


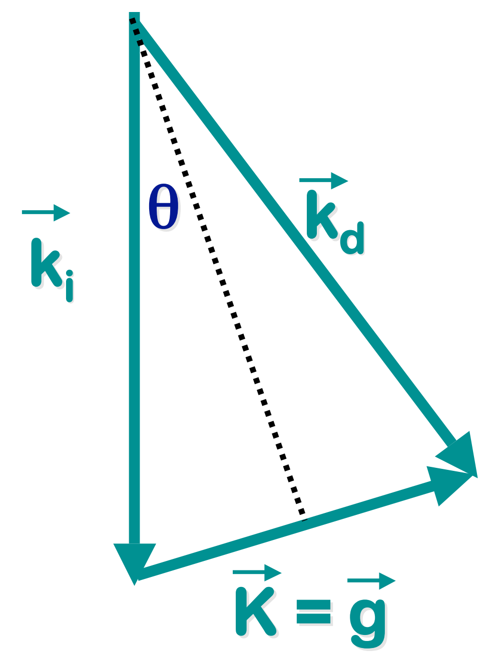
a* only parallel to **a** if **a**, **b** and **c** are mutually orthogonal

Diffraction

real space vs. reciprocal space

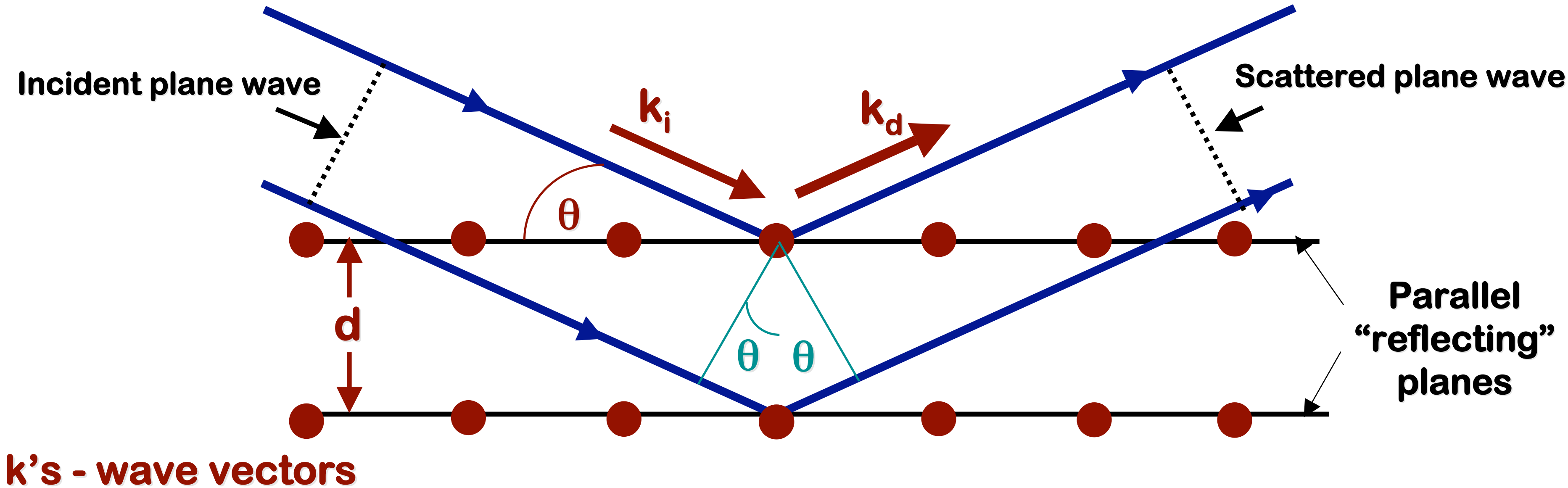


Real space

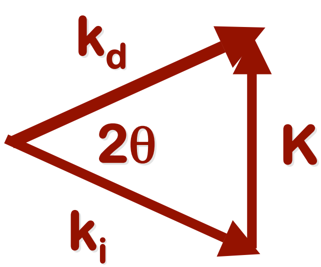


Reciprocal space

Bragg's Law



$$2d \cdot \sin\theta = n\lambda$$



$$\vec{k}_d - \vec{k}_i = \vec{K}$$

$$\left|\vec{K}\right| = \frac{2\sin\theta}{\lambda} = \frac{n}{d}$$

$$\vec{K} = \vec{g}$$

$$\left|\vec{K}\right| \propto \frac{1}{\lambda} \quad \& \quad \left|\vec{K}\right| \propto \frac{1}{d}$$

Laue Equations & Bragg's Law

Laue Equations have sol^n:

$$\vec{K} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* = \vec{g}$$

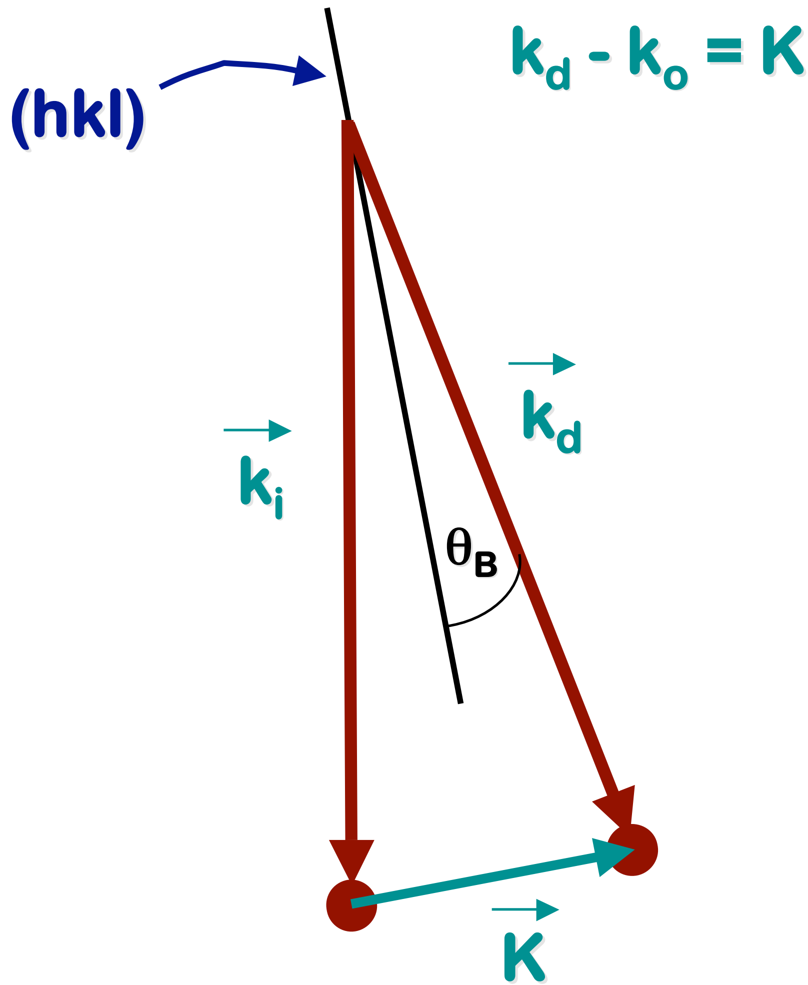
We have shown that:

$$\left|\vec{K}\right| = \frac{2\sin\theta_B}{\lambda} \quad \& \quad \left|\vec{g}\right| = \frac{1}{d_{hkl}}$$

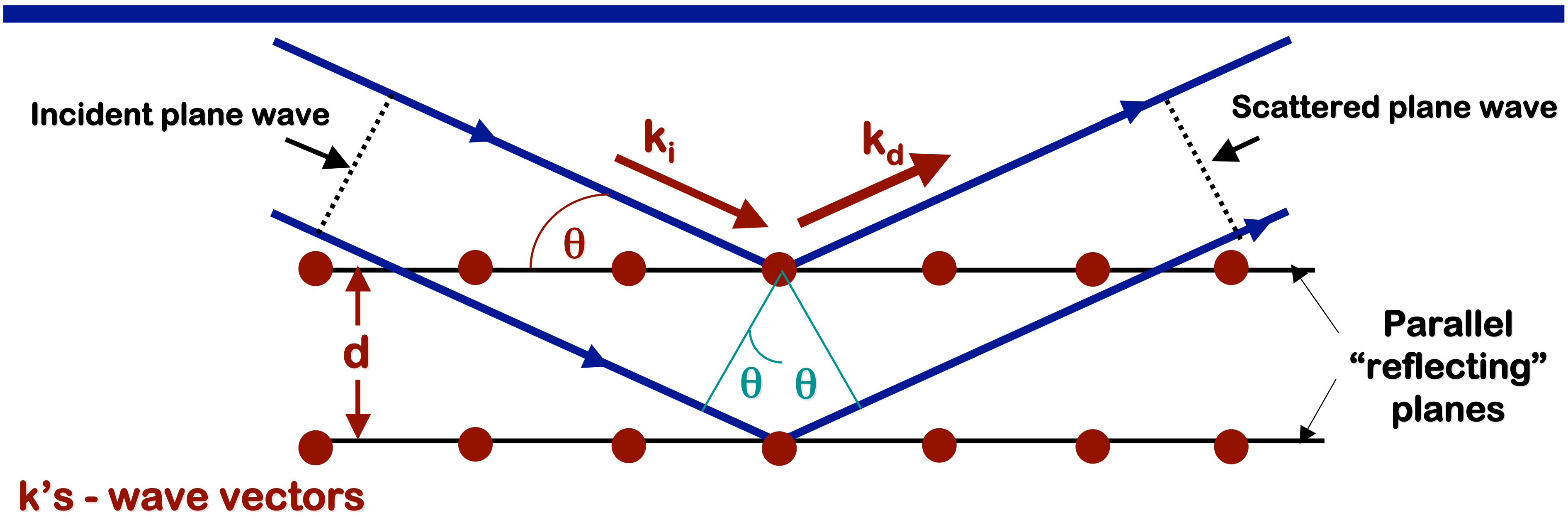
We recover Bragg's Law:

$$\frac{2\sin\theta_B}{\lambda} = \frac{1}{d_{hkl}}$$

$$2d_{hkl}\sin\theta_B = \lambda$$



Bragg's Law



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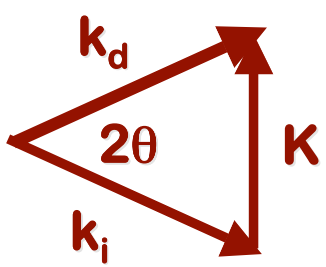

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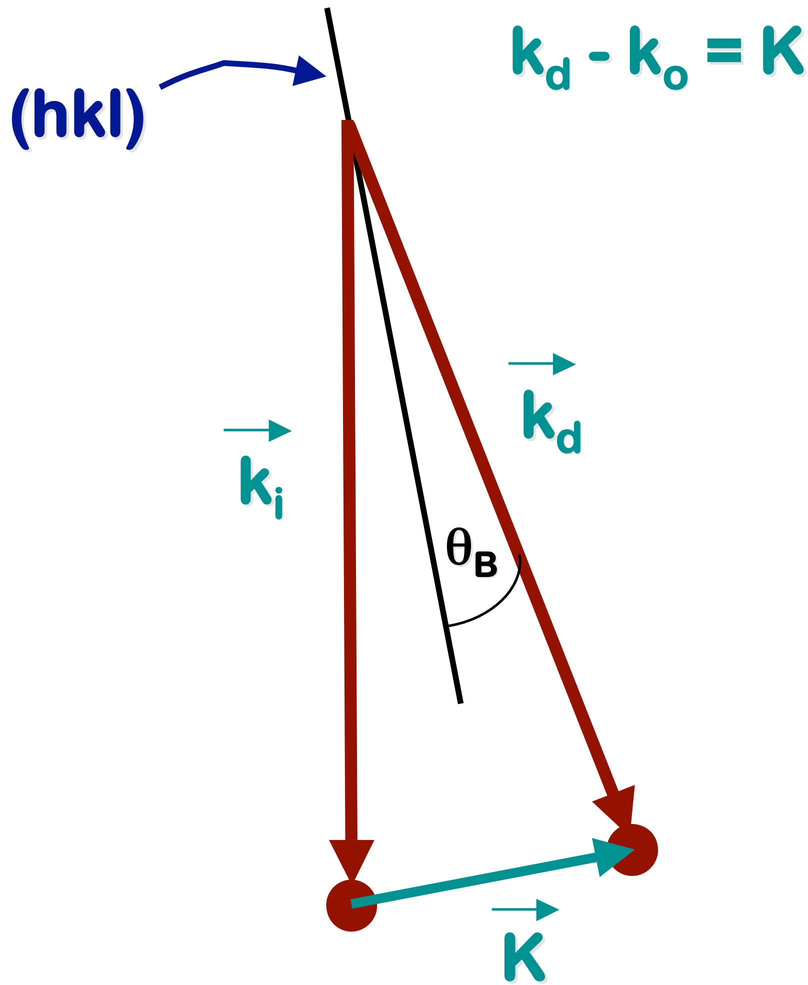
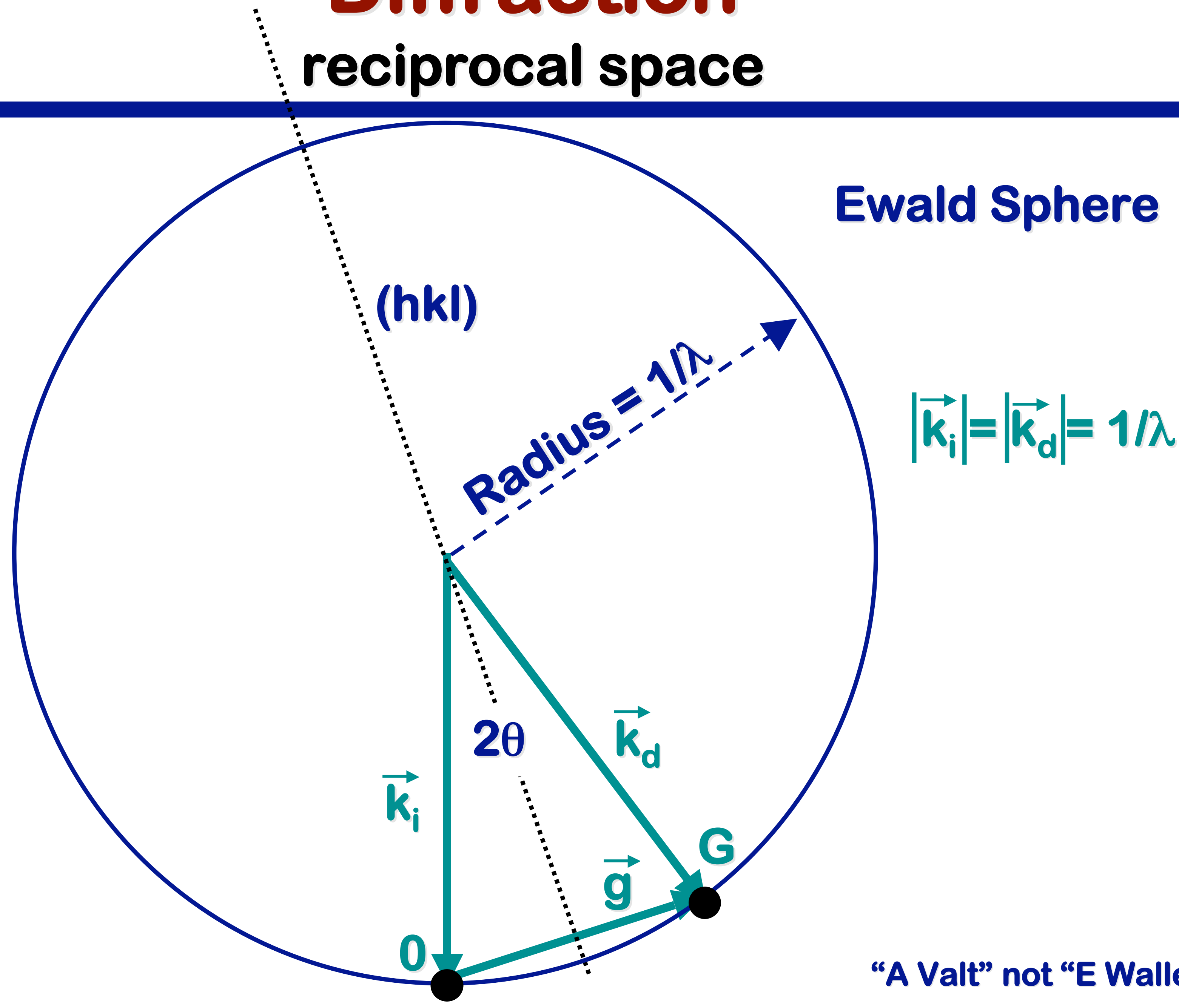


Diffraction

reciprocal space



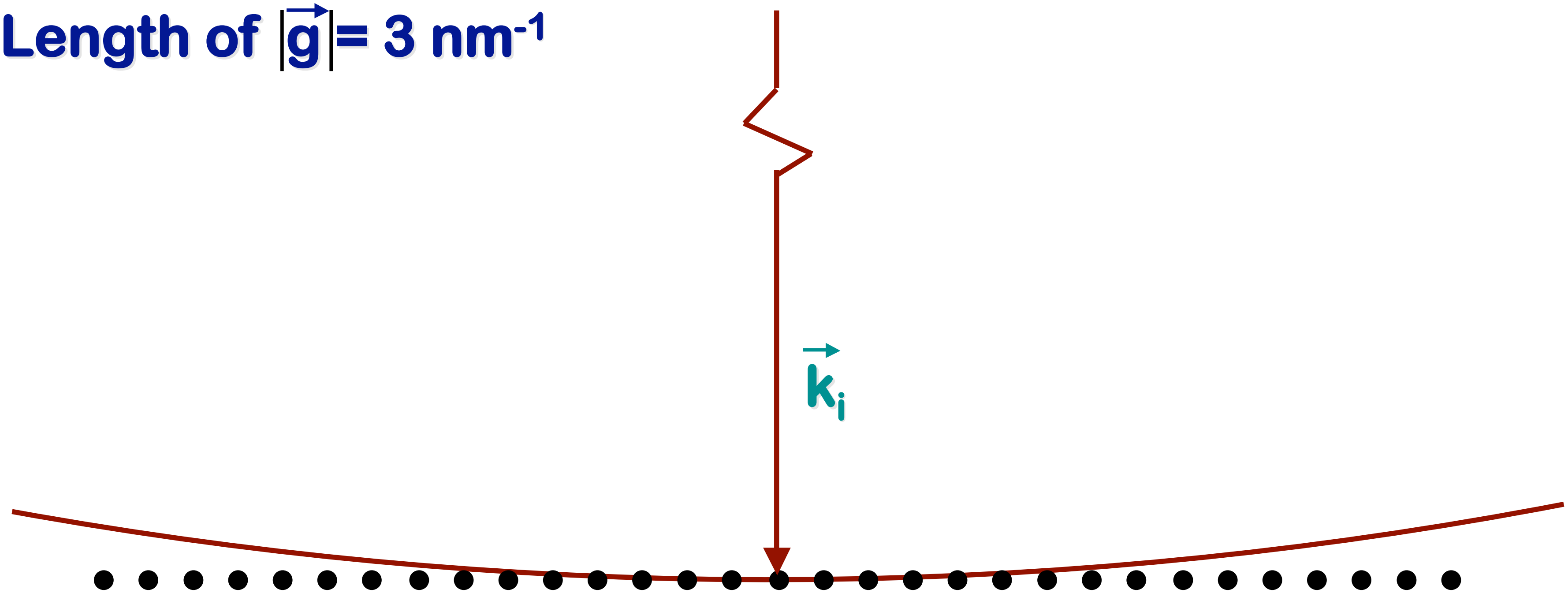
"A Valt" not "E Walled"

Diffraction

Diffraction occurs when the Ewald sphere intersects a reciprocal lattice vector

For 200 kV electrons, $1/\lambda = 1/0.00273$ nm = 366 nm^{-1}

Length of $|\vec{g}|$= 3 nm^{-1}



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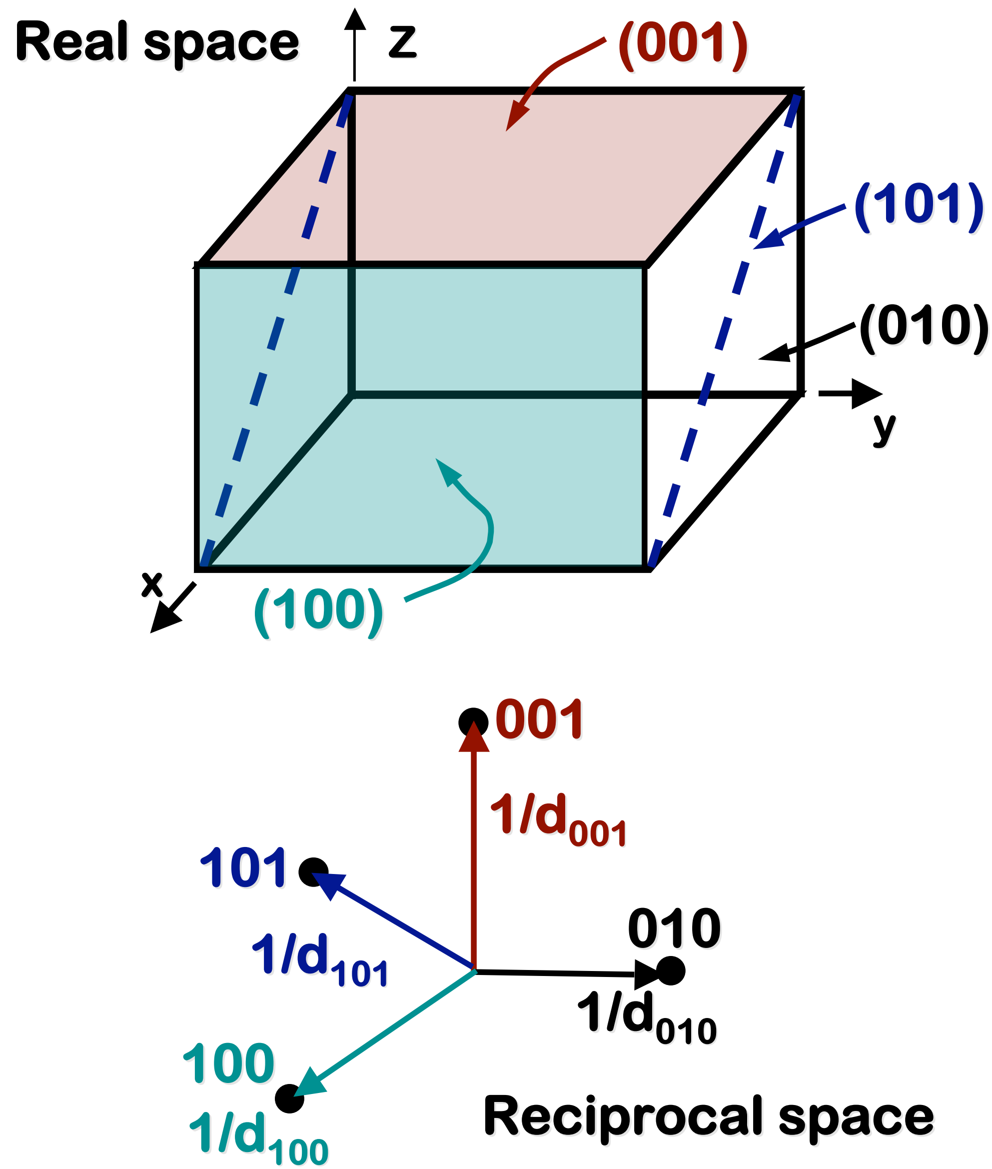

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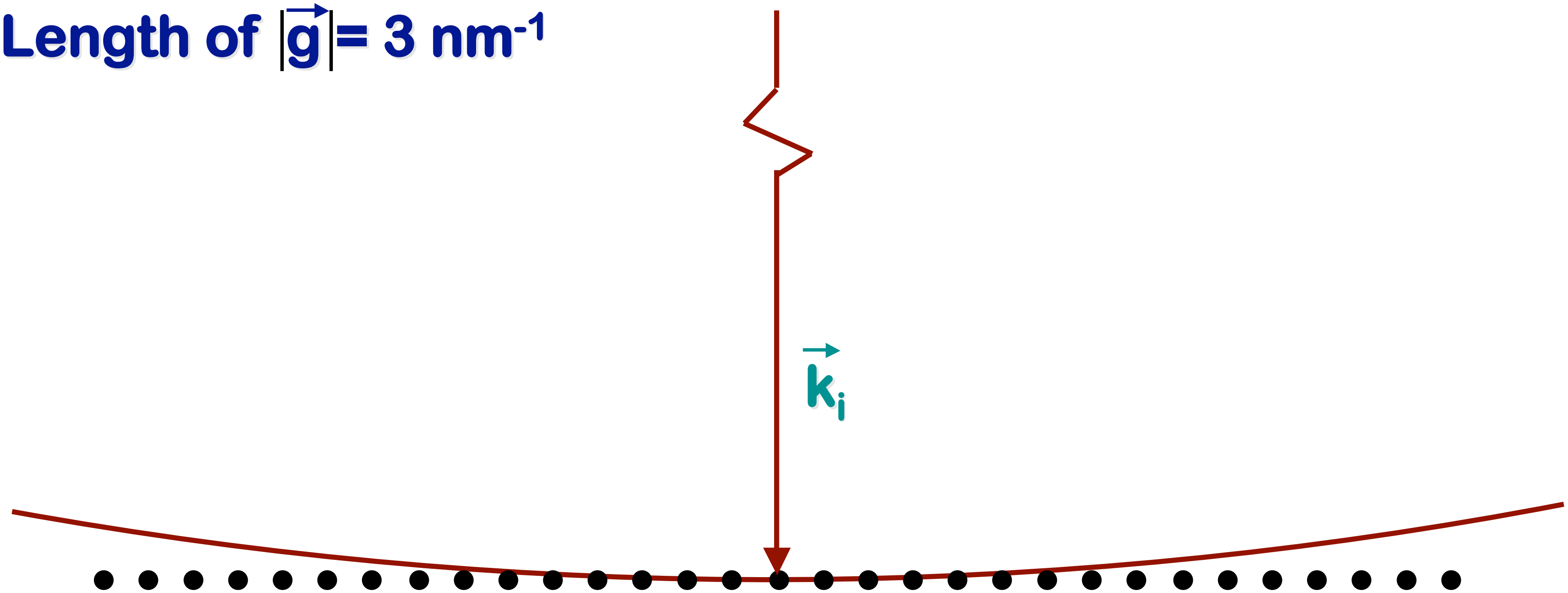

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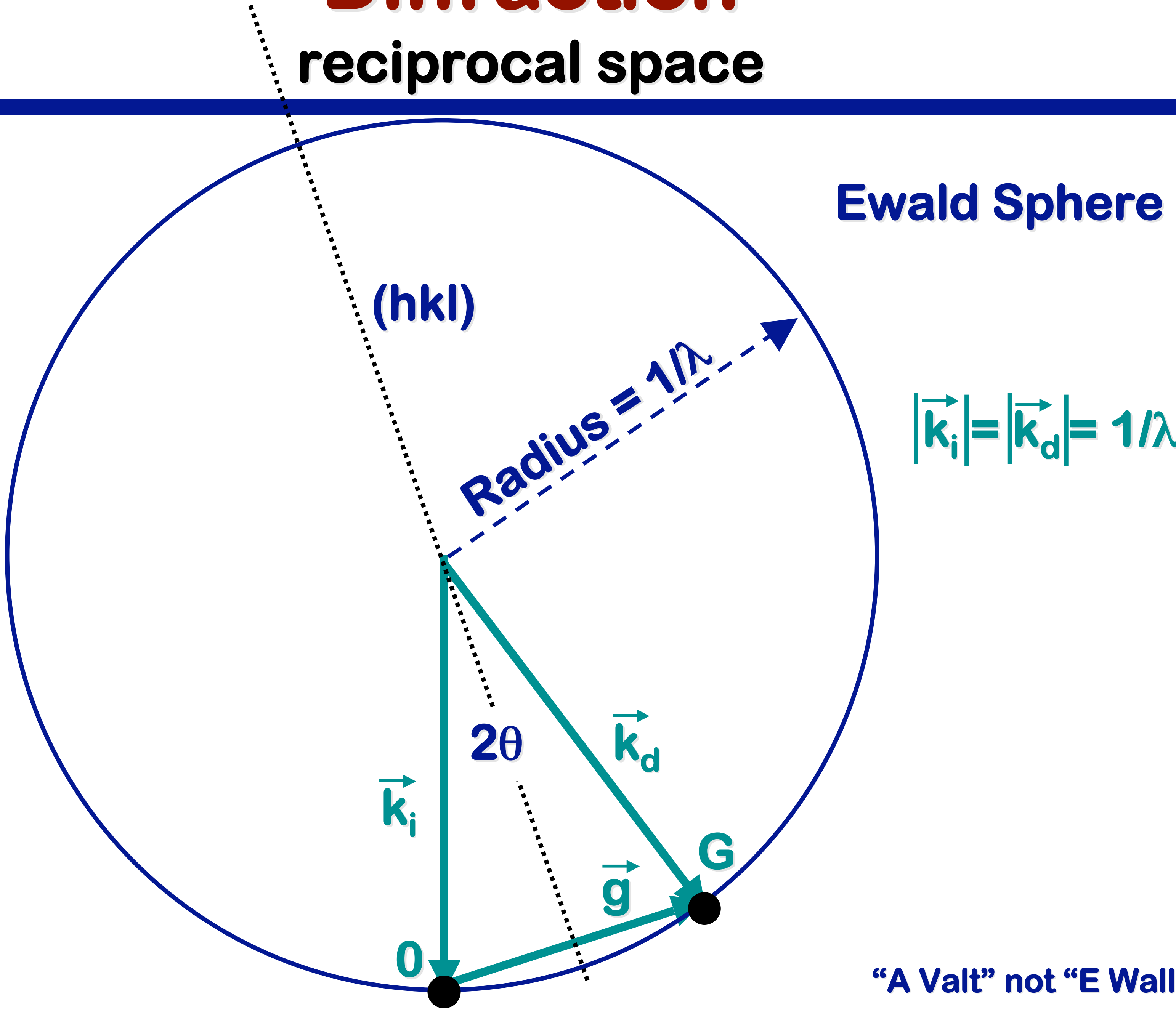

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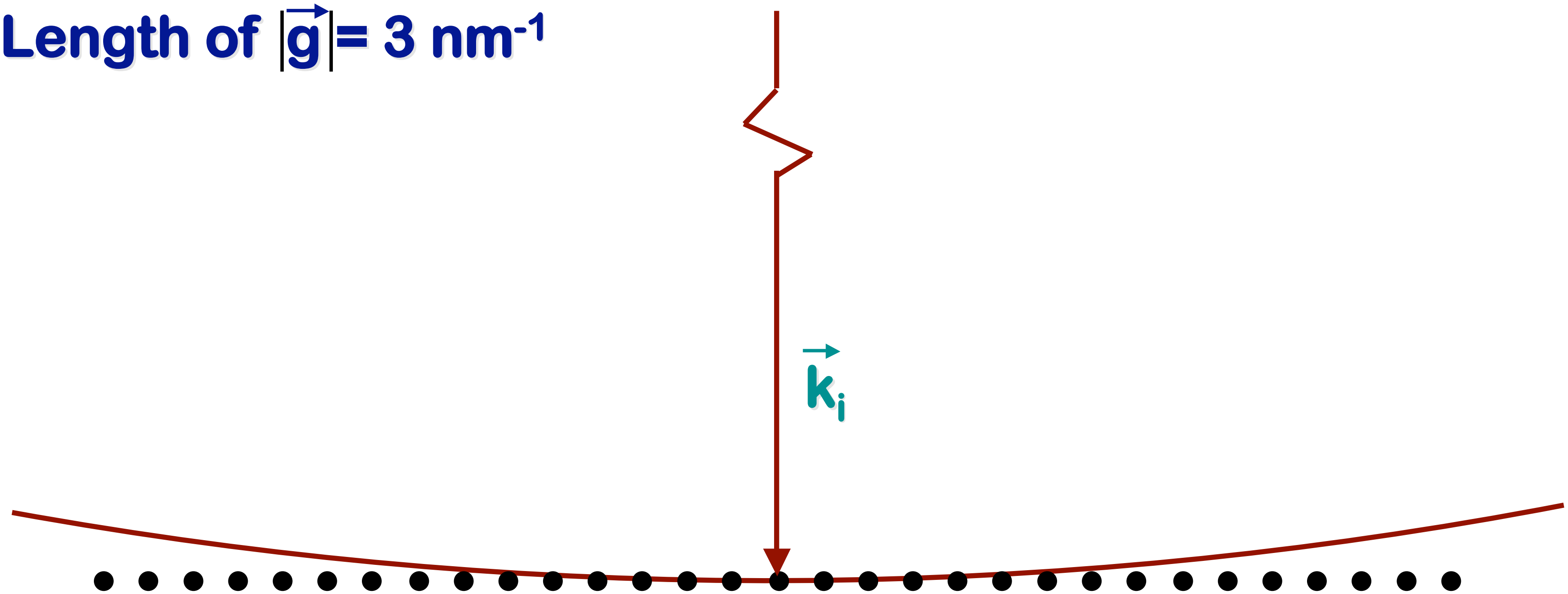
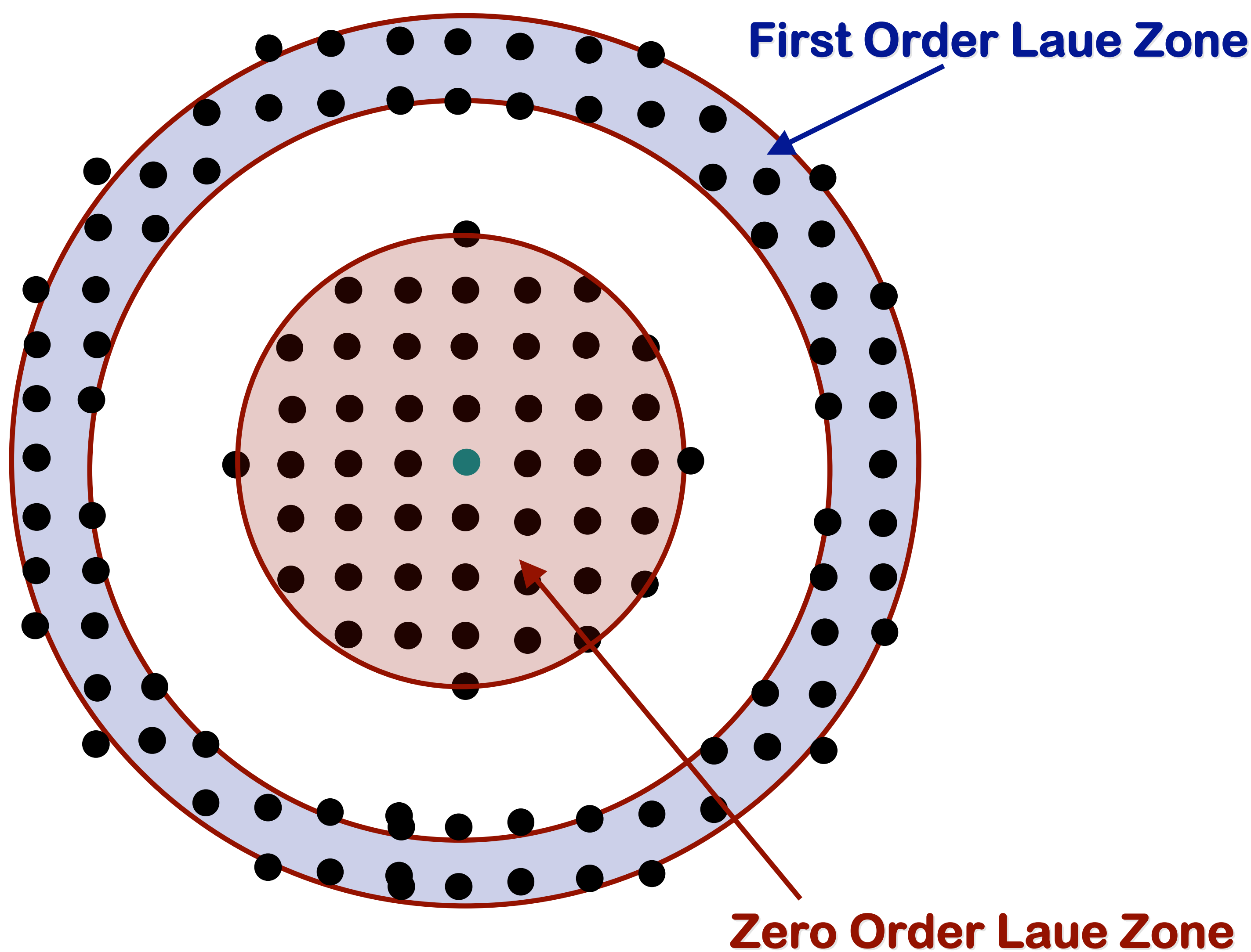


Resulting diffraction pattern



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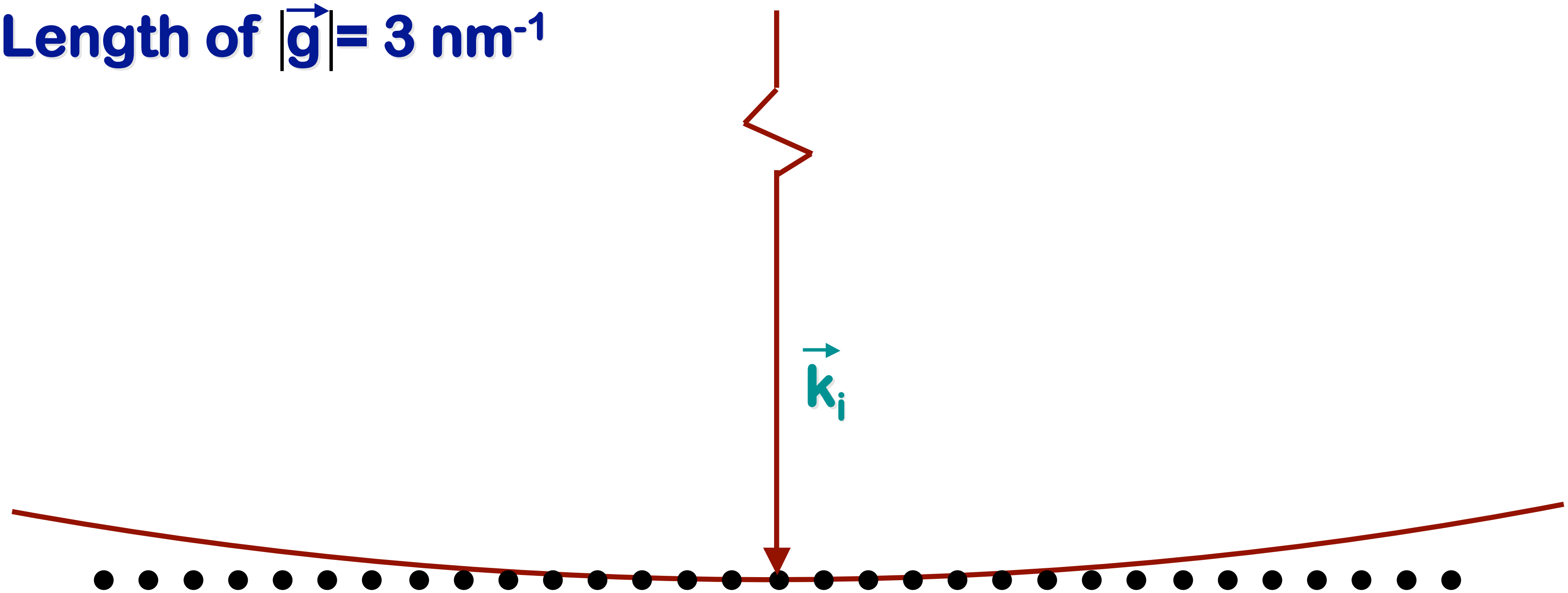
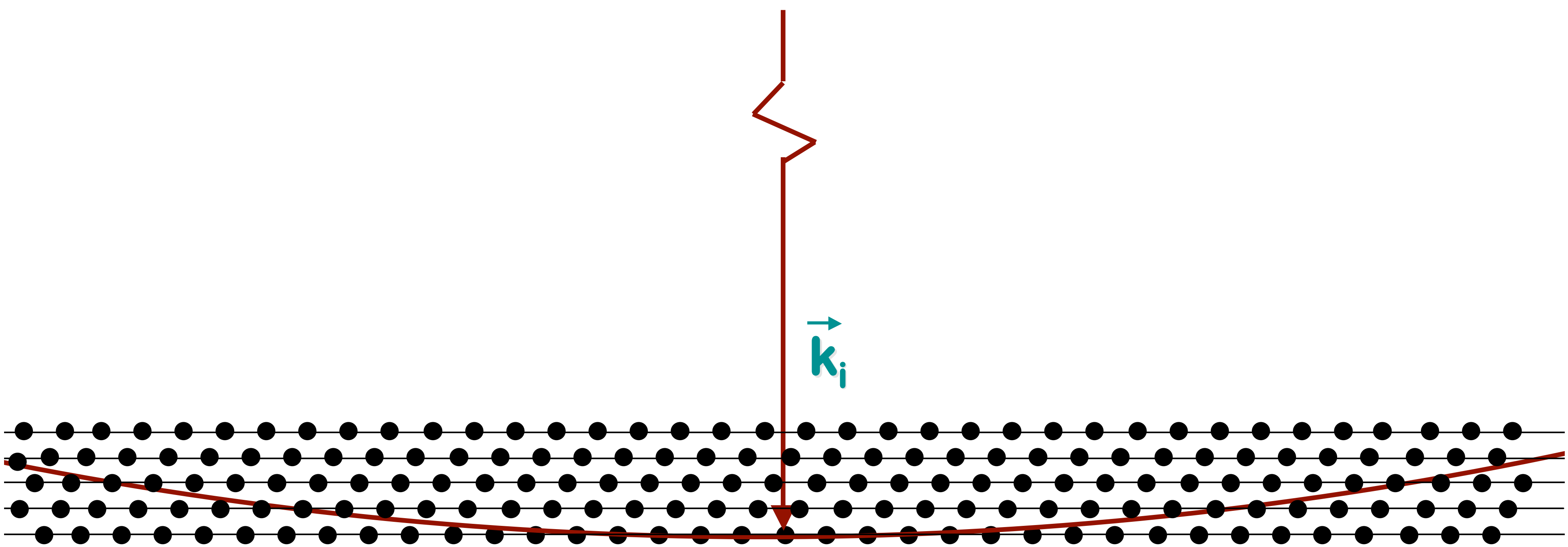


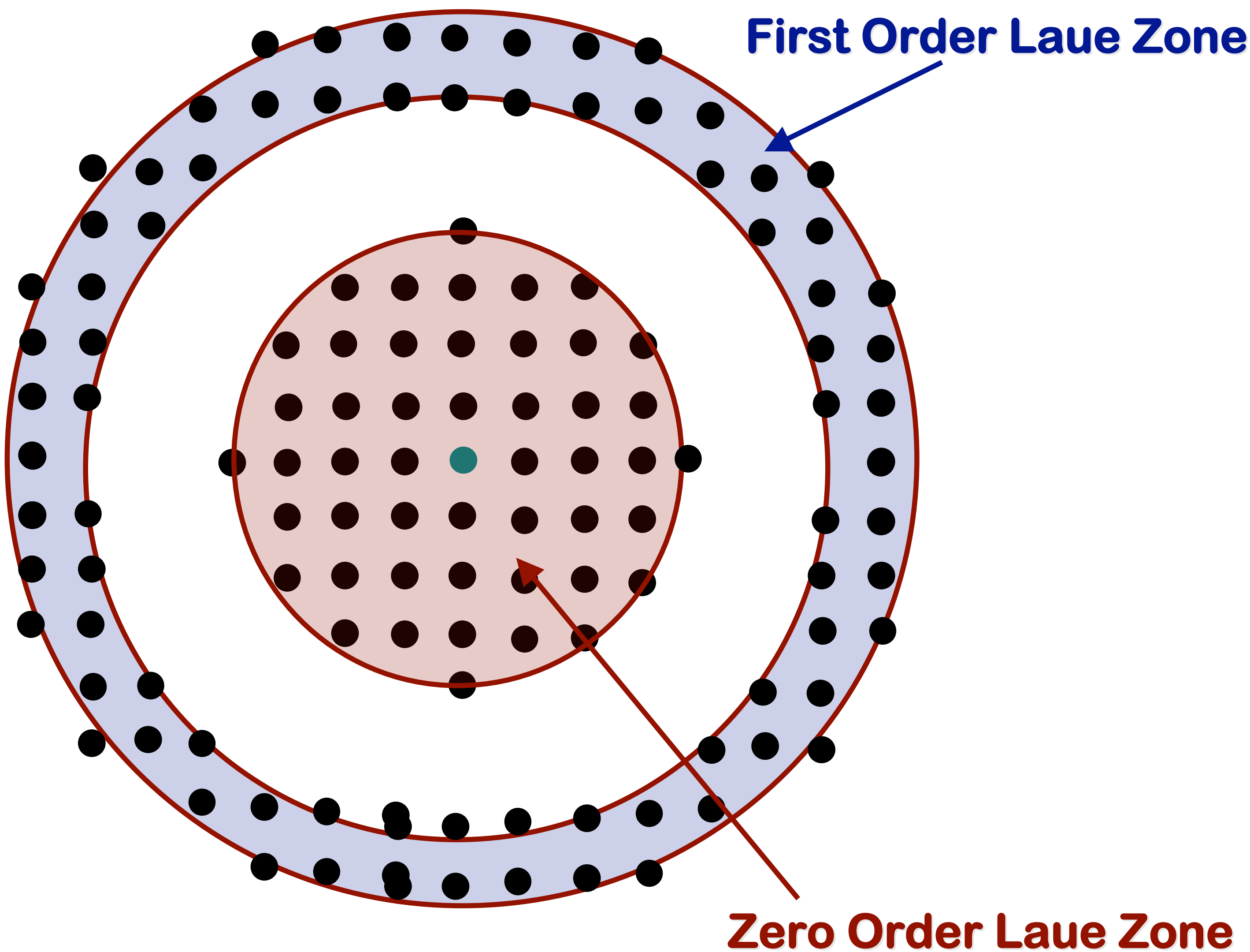
Higher order Laue Zones

Reciprocal lattice is not planar -- it is a true 3-D lattice

Zero order Laue Zone (ZOLZ), First Order Laue Zone (FOLZ), Higher order Laue Zone (HOLZ)

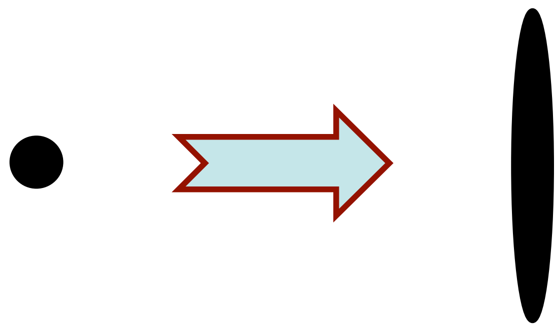


Resulting diffraction pattern



Reciprocal Lattice Rods

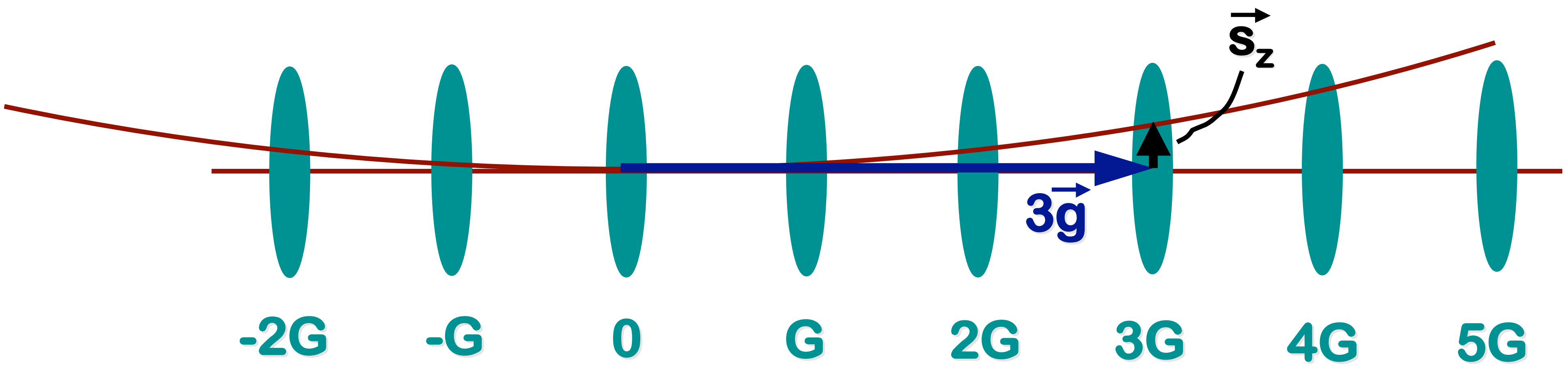
- **Each point in reciprocal space contains not a point, but rather a rod - “rel-rod”**
  - Result of the finite size of our diffracting crystals
  - We’ll derive this in a couple of lectures: for now, just believe me!



Ewald Sphere and Rel-rods

Presence of rel-rods "relaxes" diffraction requirements

New vector - $\vec{s}$ - called "deviation parameter"



Resulting diffraction pattern