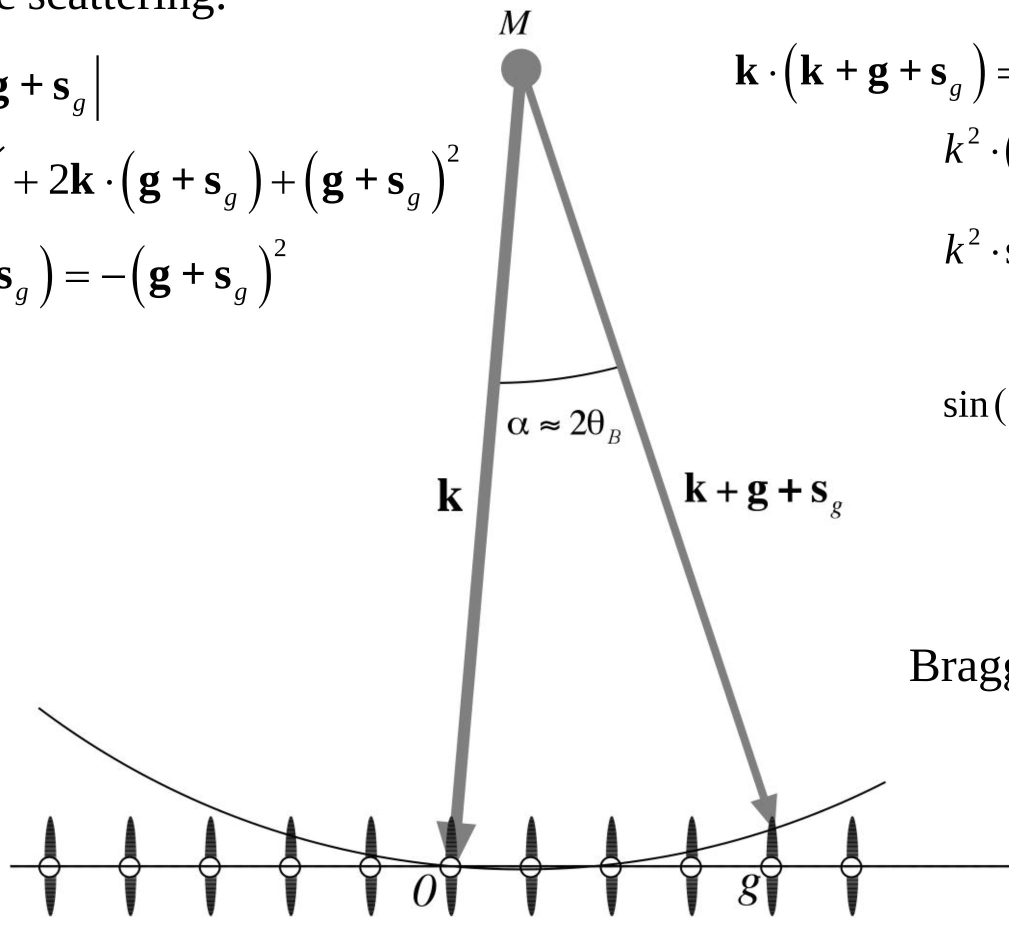
Changes in diffraction angle

Elastic scattering:

$$k = \left|\mathbf{k} + \mathbf{g} + \mathbf{s}_g\right|$$

$$\cancel{k^2} = \cancel{k^2} + 2\mathbf{k}\cdot\left(\mathbf{g} + \mathbf{s}_g\right) + \left(\mathbf{g} + \mathbf{s}_g\right)^2$$

$$2\mathbf{k}\cdot\left(\mathbf{g} + \mathbf{s}_g\right) = -\left(\mathbf{g} + \mathbf{s}_g\right)^2$$



Find diffraction angle:

$$\mathbf{k}\cdot\left(\mathbf{k} + \mathbf{g} + \mathbf{s}_g\right) = k^2 \cos\alpha = k^2 + \mathbf{k}\cdot\left(\mathbf{g} + \mathbf{s}_\mathbf{g}\right)$$

$$k^2 \cdot (1 - \cos\alpha) = -\mathbf{k}\cdot\left(\mathbf{g} + \mathbf{s}_\mathbf{g}\right)$$

$$k^2 \cdot \sin^2(\alpha/2) = \frac{1}{2}\left(\mathbf{g} + \mathbf{s}_\mathbf{g}\right)^2$$

$$\sin(\alpha/2) = \frac{1}{2k}\sqrt{g^2 + 2\,\cancel{\mathbf{g}\cdot\mathbf{s}_\mathbf{g}} + s_\mathbf{g}^2}$$

$$\alpha = 2\cdot\sin^{-1}\left[\frac{g}{2k}\sqrt{1 + \left(\frac{s_\mathbf{g}}{g}\right)^2}\right]$$

Bragg's Law: $\frac{g}{2k} = \sin\theta_B$

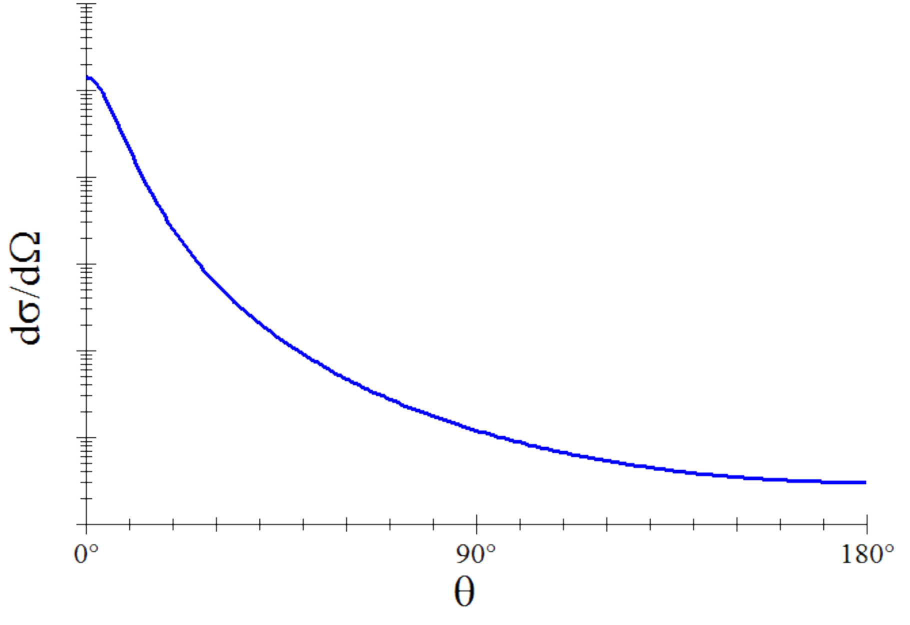
Small-angles:

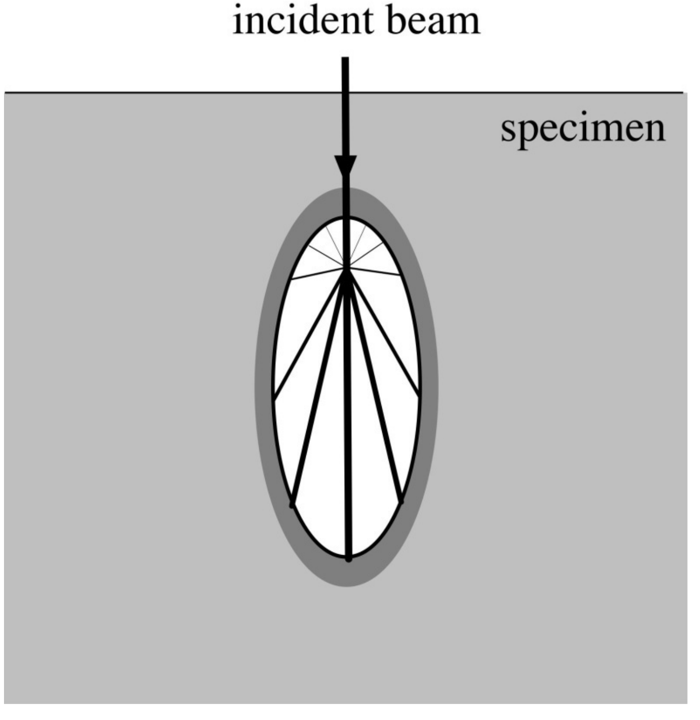
$$\alpha \approx 2\theta_B \cdot \left[1 + \frac{1}{2}\left(\frac{s_g}{g}\right)^2\right]$$

Diffraction angle almost unaffected by sample tilt.

Incoherent, diffuse scattering

Elastic scattering occurs in all directions, but primarily forward.
Multiple scattering events result in incoherent, diffuse electrons



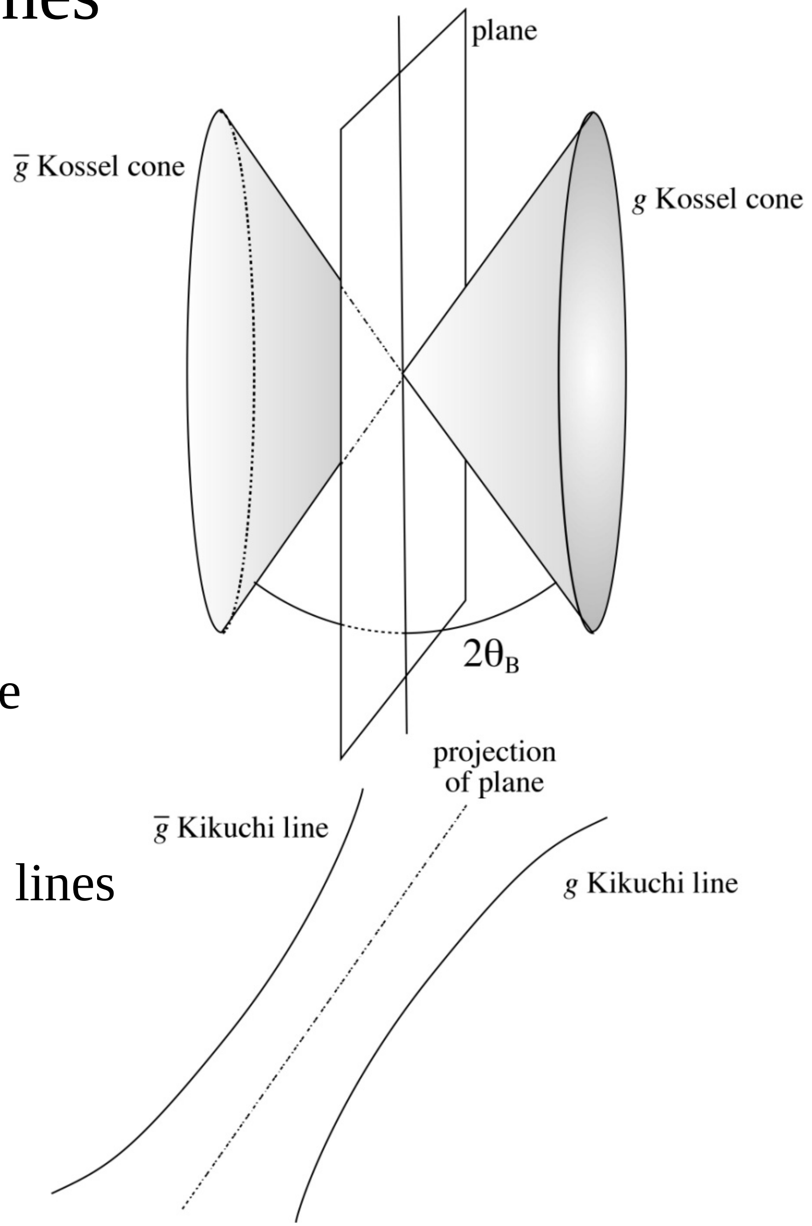


Kossel cones

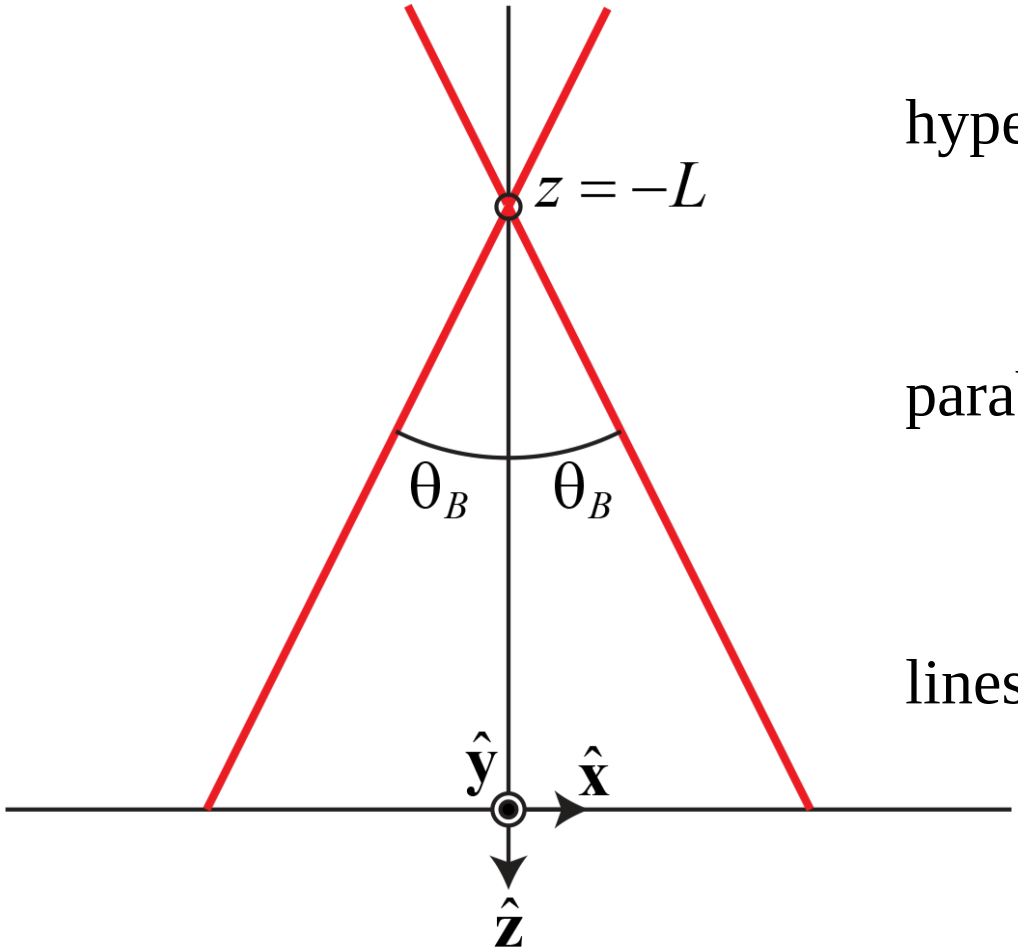
Diffuse scattering off (*hkl*)
creates cones at $\pm\theta_B$ from plane

Intersection of cone with projection plane
traces a hyperbola

At small angles the hyperbolas appear as lines



Kossel cone construction



cones:

$$\frac{x}{\tan\theta_B} = \pm\sqrt{y^2 + (z+L)^2}$$

hyperbolas @ z=0:

$$x = \pm\tan\theta_B\sqrt{y^2 + L^2}$$

parabolas for small y:

$$x \approx \pm L\cdot\tan\theta_B\cdot\left(1+\frac{y^2}{2L^2}\right)$$

lines for very small y:

$$x \approx \pm L\cdot\tan\theta_B$$

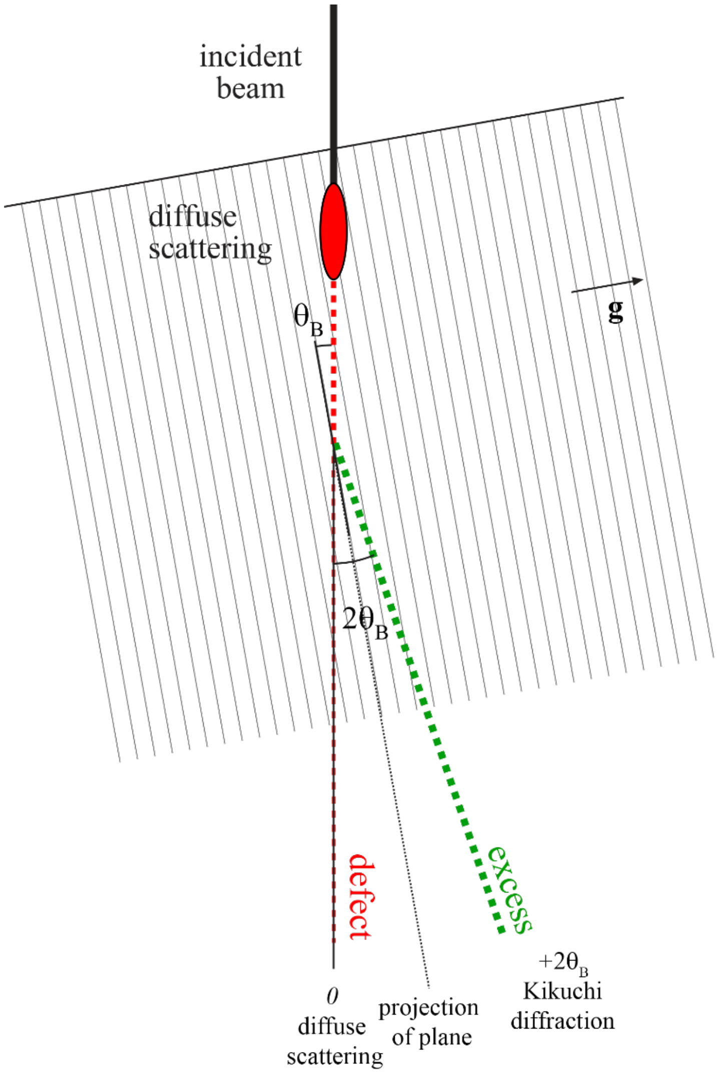
Kikuchi diffraction

Sequence of:
1) incoherent, diffuse scattering followed by
2) coherent elastic scattering

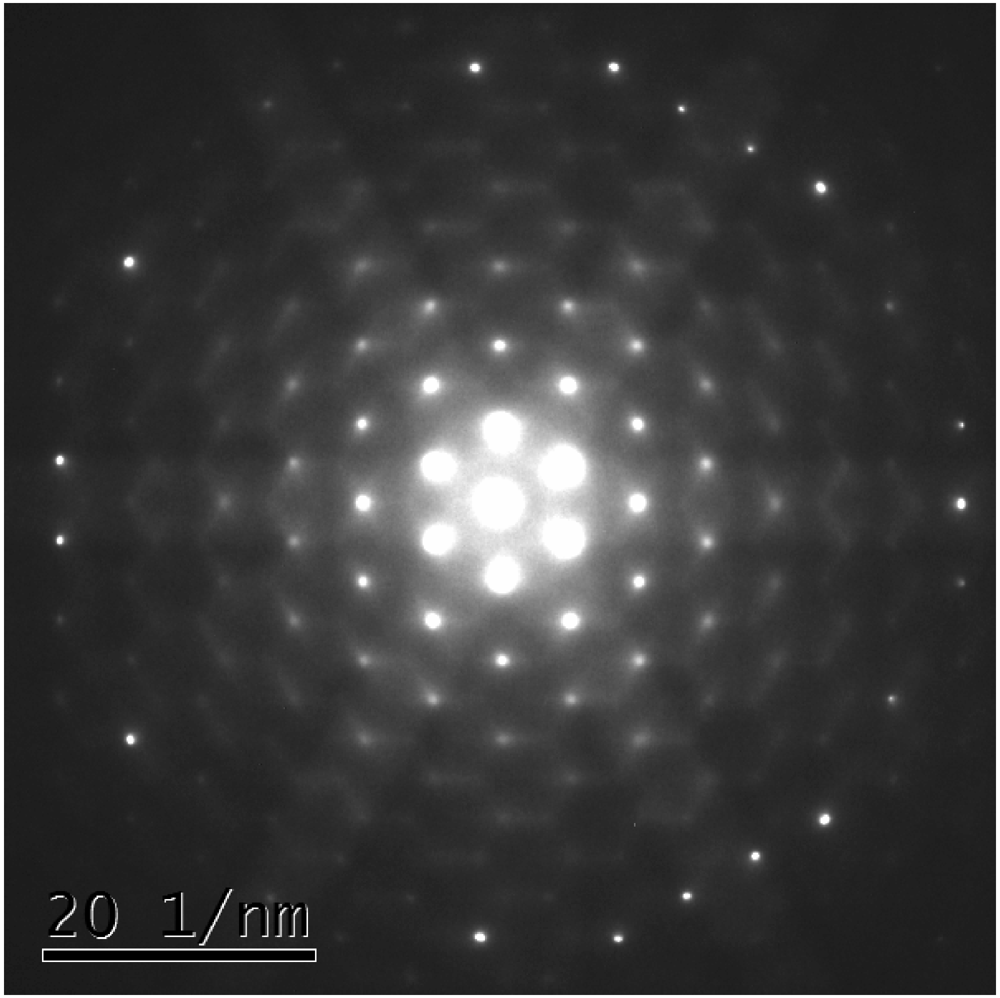
Diffuse scattering strongest in forward direction

At Bragg condition:

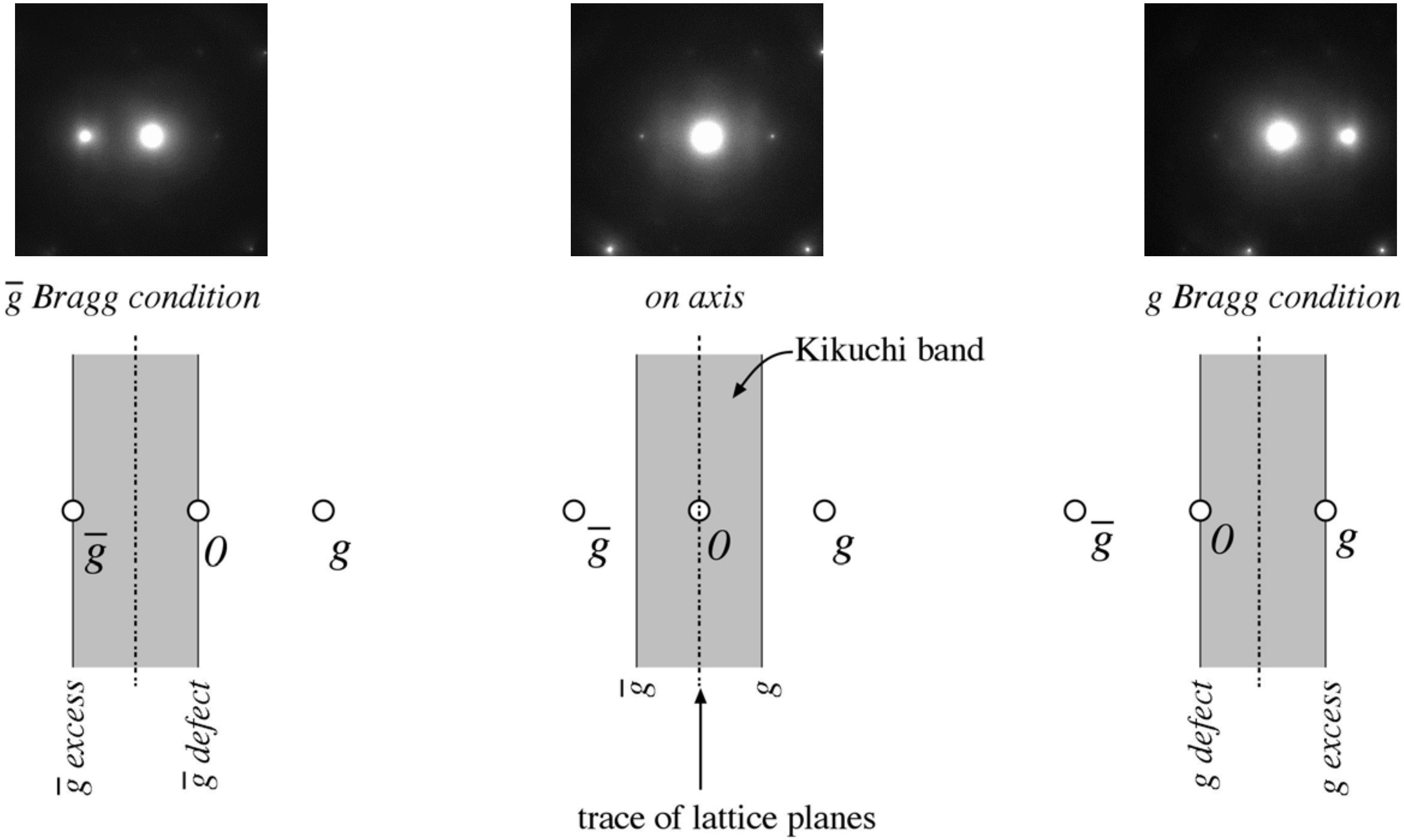
→ dark (defect) line at 0°
→ bright (excess) line at $2\theta_B$



Example: Si<111>



Kikuchi bands



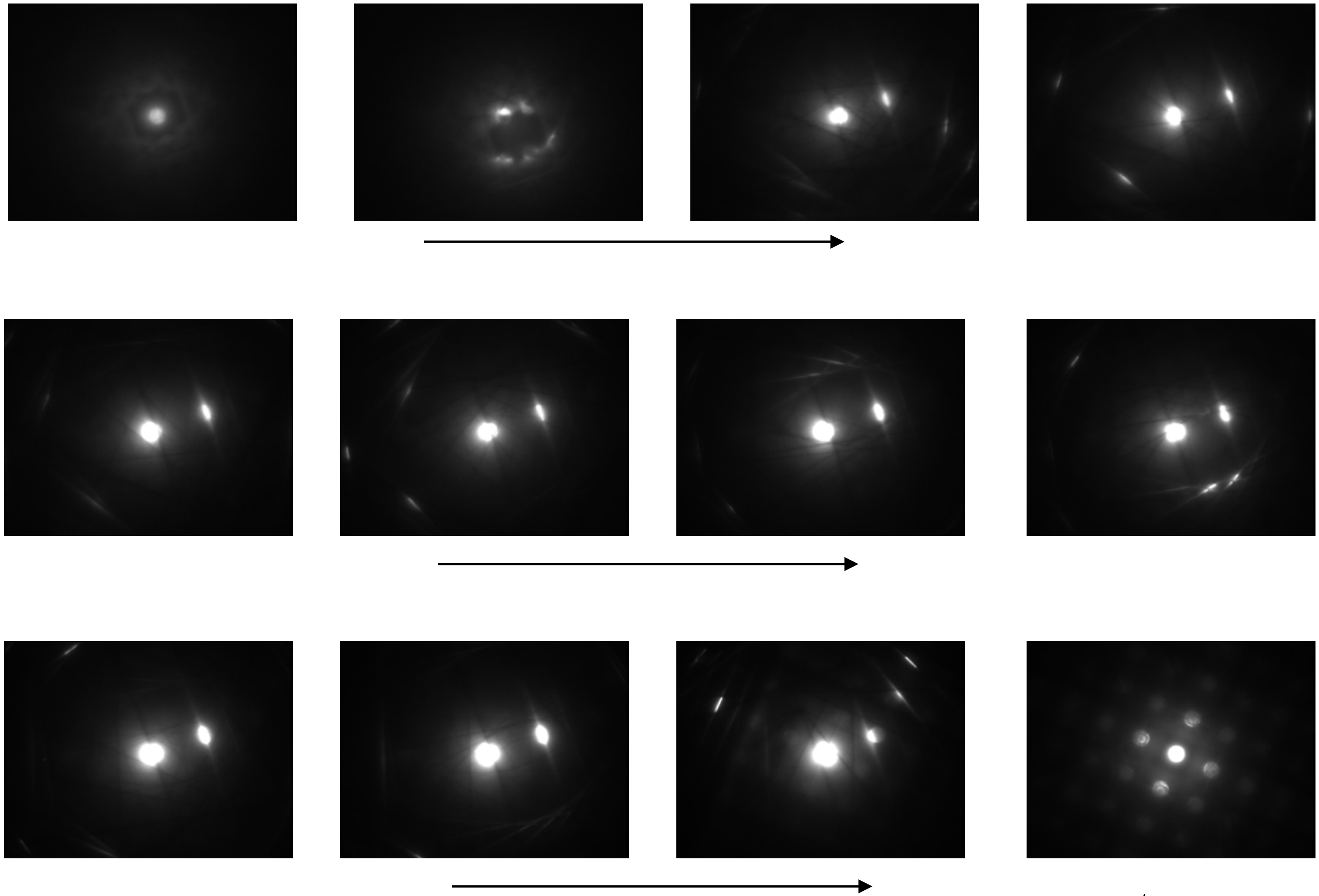
When rotating sample:

1) Bragg reflections don’t move. (They *do* change intensity.)

2) Kikuchi bands move with sample.

Tracking a Kikuchi Band

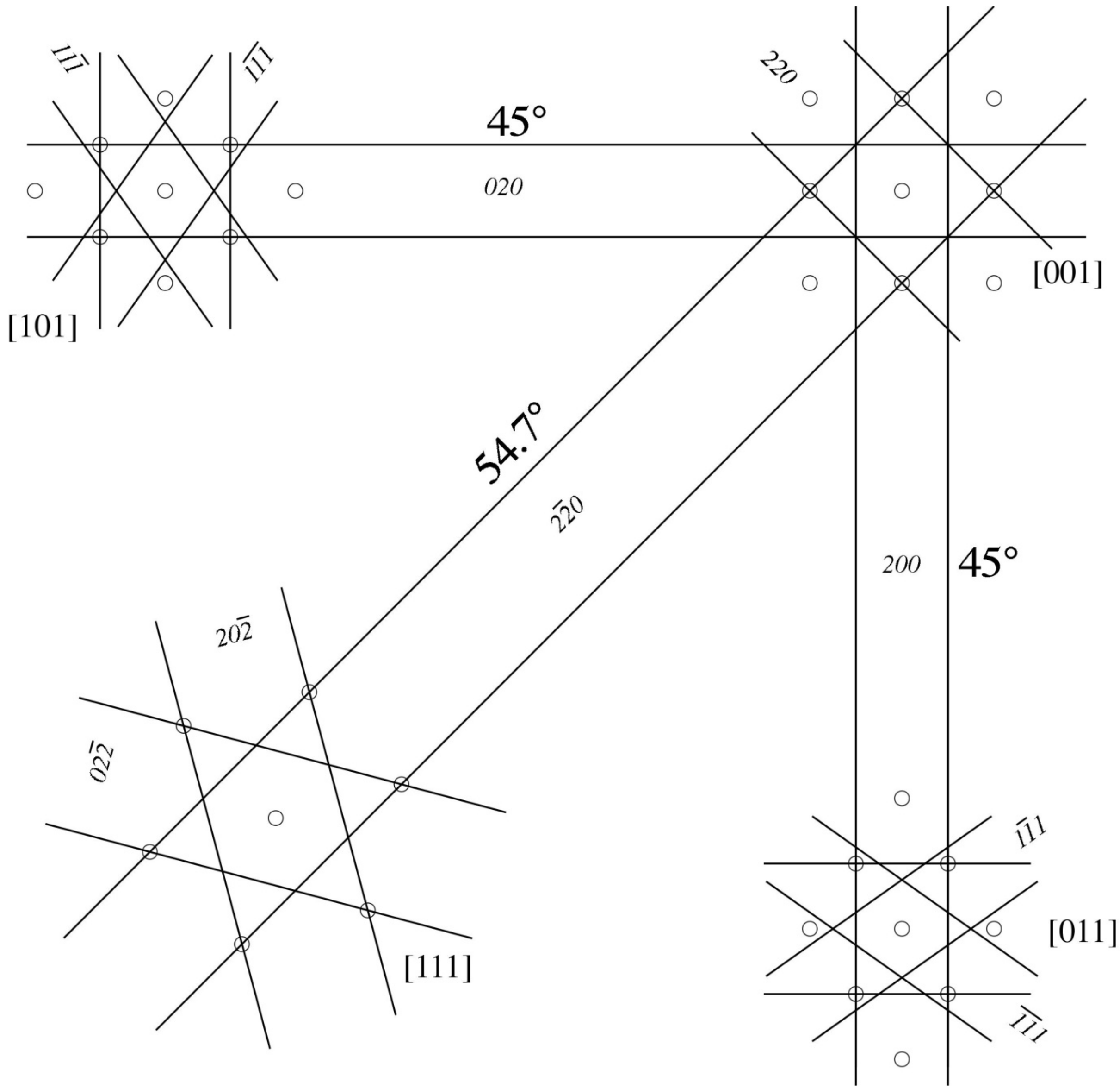
start



stop

Use to navigate among zone axes

Kikuchi Map: fcc

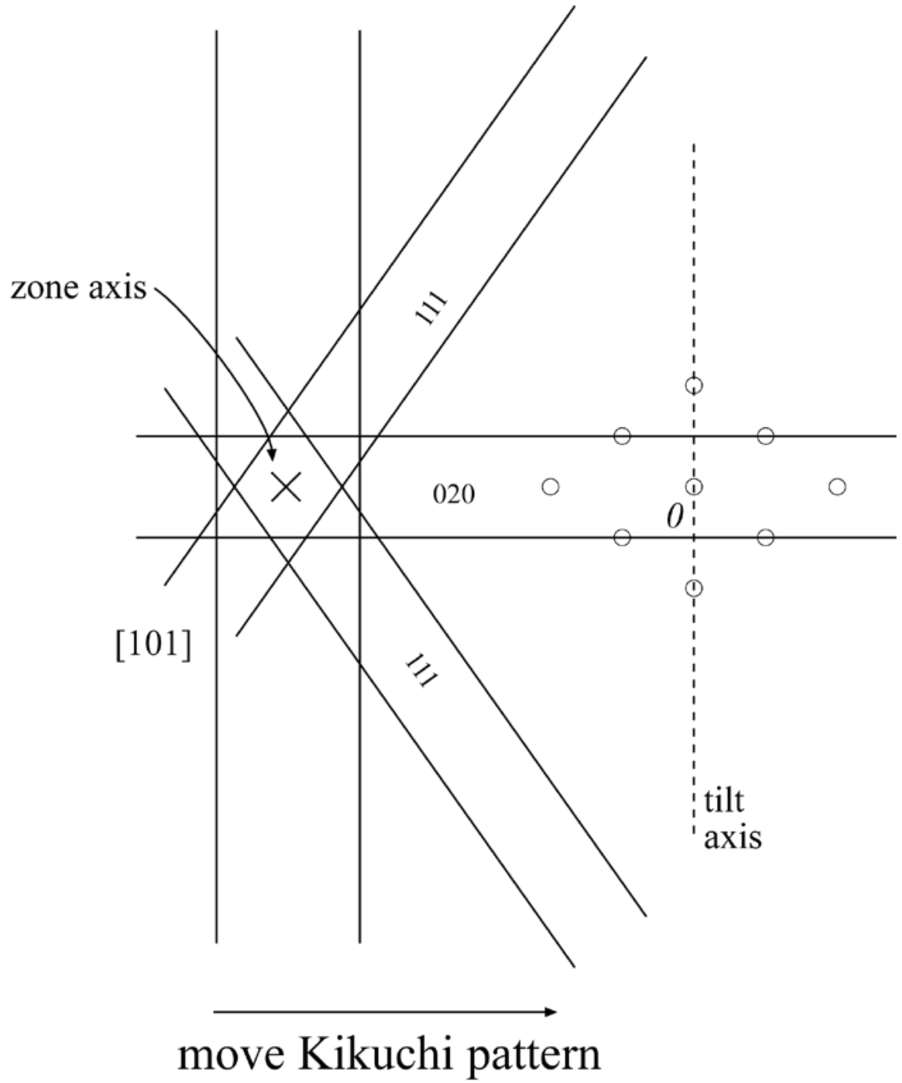


Orienting on the zone axis with Kikuchi lines

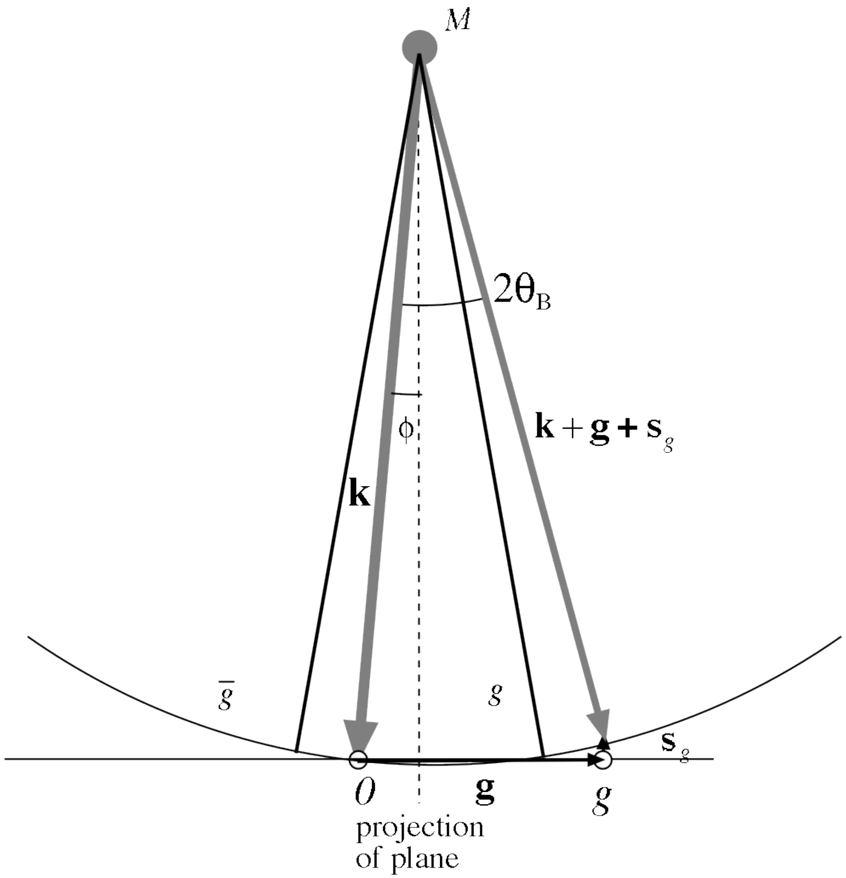
Tilt to align zone axis with direct beam

Kikuchi lines move.

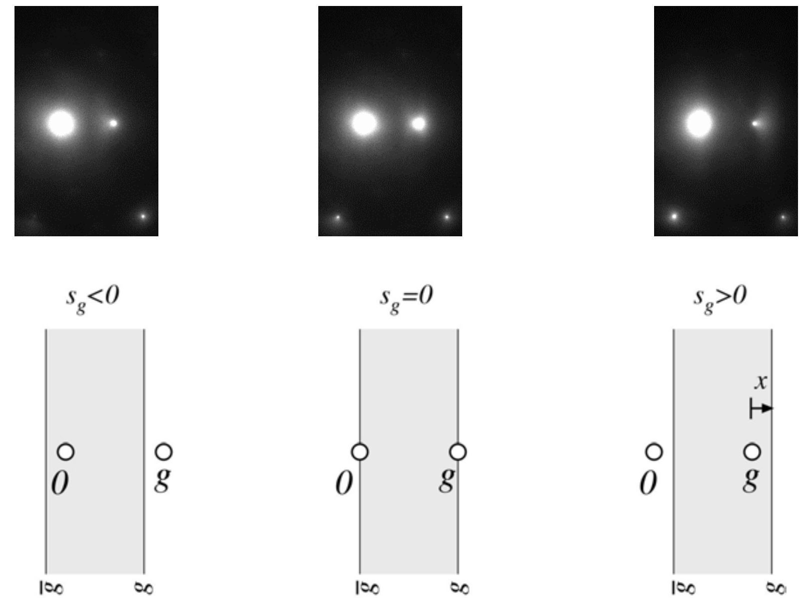
Diffraction spots stay fixed.



Measuring s_g



$x<0$



Estimate tilt:

$$\phi = \theta_B \cdot \left(\frac{2x}{g}+1\right) = \frac{g}{2k}\cdot\left(\frac{2x}{g}+1\right) = \frac{x}{k}+\frac{g}{2k}$$

Small angles:

$$s \approx g\phi - \frac{g^2}{2k} = g\cdot\left(\frac{x}{k}+\cancel{\frac{g}{2k}}\right) - \cancel{\frac{g^2}{2k}}$$

$$\Rightarrow s = \frac{gx}{k}$$