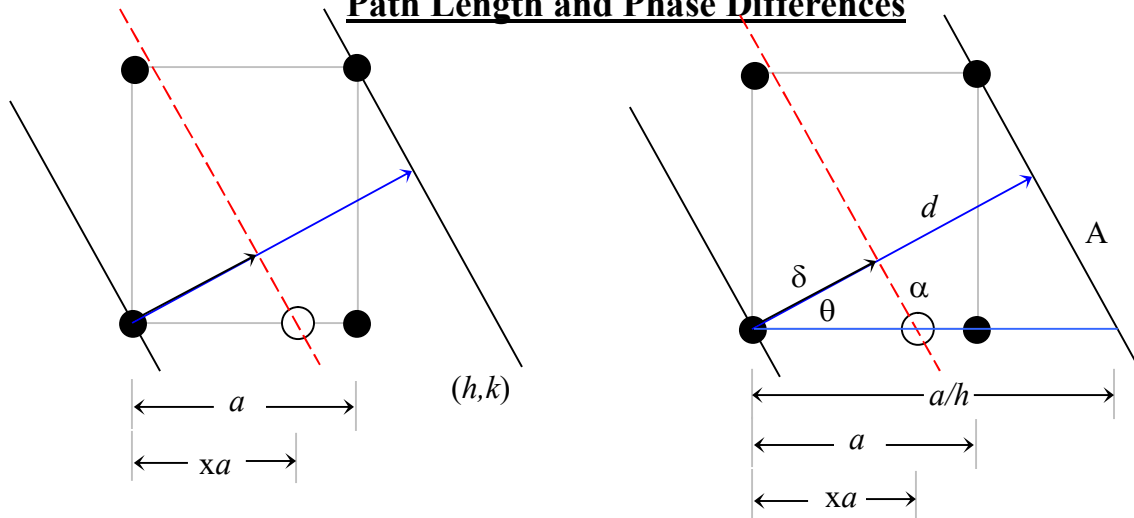


Path Length and Phase Differences



Unit cell side = a

Set of diffraction planes = (h,k)

New atom in unit cell at position = xa

Path length difference for rays reflecting from old and new planes = δ

for large Δ : $d^2 = \frac{a^2}{h^2} - A^2$

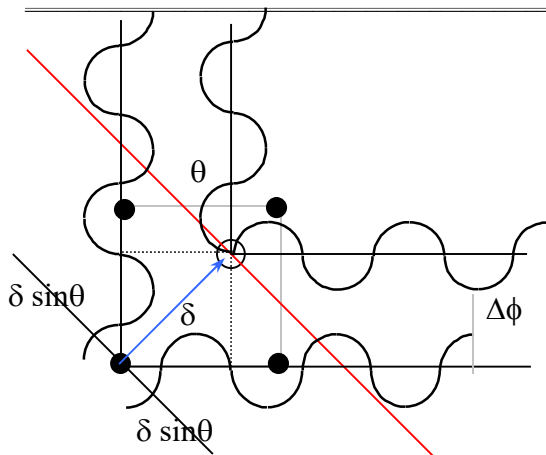
for small Δ : $\delta^2 = x^2 a^2 - \alpha^2$

$\alpha = xa \sin \theta$ $A = \frac{a}{h} \sin \theta$

$\delta^2 = x^2 a^2 (1 - \sin^2 \theta)$
 $d^2 = \frac{a^2}{h^2} (1 - \sin^2 \theta)$

} $\frac{\delta}{d} = \frac{xa}{\frac{a}{h}} = hx$

$\delta = (hx) d$ in general: $\delta = (hx + ky + lz) d$



diffraction angle: $2 d \sin \theta = \lambda$
 $\sin \theta = \lambda/2d$

extra path length: $\Delta x = 2 \delta \sin \theta = \delta \lambda/d$

phase difference: $\Delta x \frac{2\pi}{\lambda} = 2\pi \frac{\delta}{d}$

phase difference: $\Delta \phi = 2\pi (hx + ky + lz)$

plane wave amplitude: $e^{2\pi i (hx + ky + lz)}$