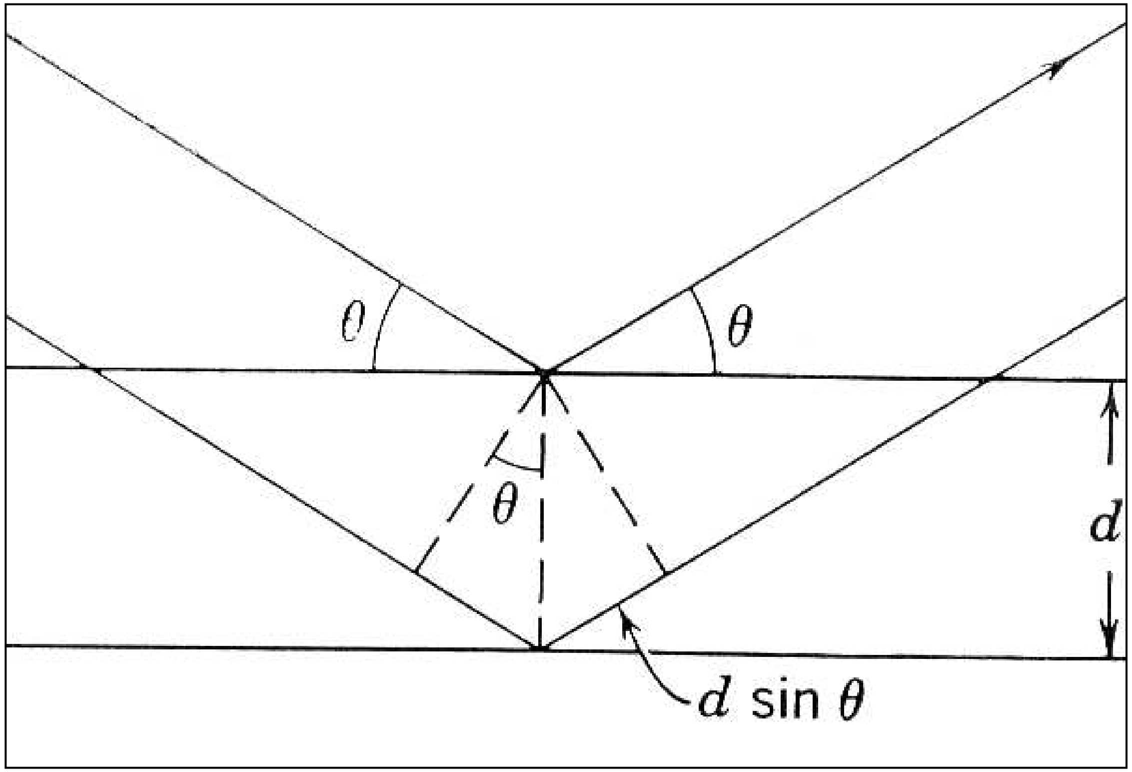
Week 3

- Bragg reflection
- Laue conditions
- Bonding in crystals
- Phonons

Diffraction of x-rays
Bragg's law (1913)

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

n-th order reflection from the (h,k,l) plane



Laue condition

$\hbar\mathbf{k}$ momentum of incident photons

$\hbar\mathbf{k'}$ momentum of scattered photons

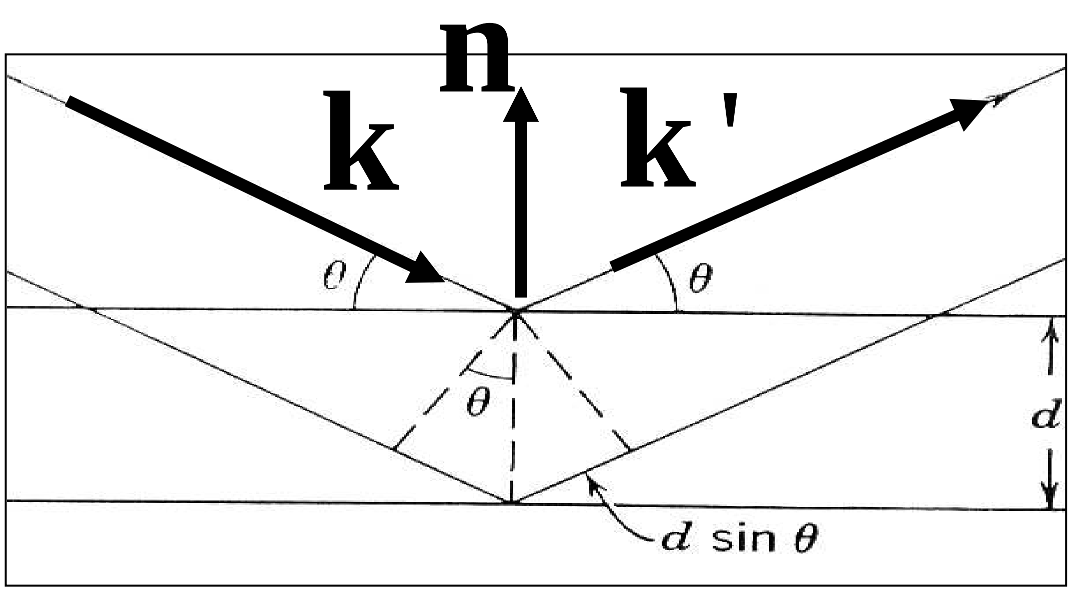
$\mathbf{Q} = \mathbf{k'} - \mathbf{k}$ scattering vector

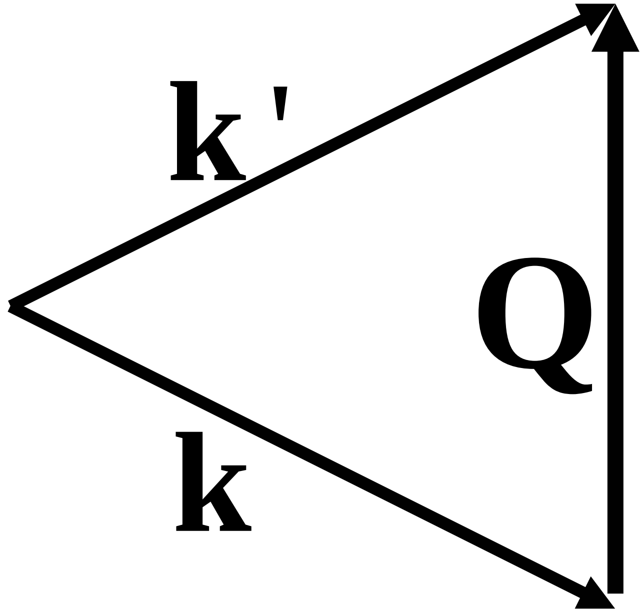
$$2d_{h,k,l}\sin\theta = n\lambda \qquad 2\frac{2\pi}{\lambda}\sin\theta = n\frac{2\pi}{d_{h,k,l}}$$

$$\frac{2\pi}{\lambda} = k \qquad 2k\sin\theta = |\mathbf{k} - \mathbf{k}'| = |\mathbf{Q}|$$

$$\frac{2\pi}{d_{h,k,l}} = |\mathbf{K}_{h,k,l}| \qquad |\mathbf{Q}| = n\,|\mathbf{K}_{h,k,l}|$$

Comparison of Bragg and Laue conditions





$$\begin{cases} |\mathbf{Q}| = n\,|\mathbf{K}_{h,k,l}| \\ \mathbf{Q} = |\mathbf{Q}|\,\mathbf{n} \\ \mathbf{K}_{h,k,l} = |\mathbf{K}_{h,k,l}|\,\mathbf{n} \end{cases} \Rightarrow \quad \mathbf{Q} = n\mathbf{K}_{h,k,l}$$

Scattering vector equals n reciprocal vectors

Bonding in crystals

- Van der Waals bonding (inert gases)
- Ionic bonding (NaCl)
- Covalent bonding (Diamond)
- Hydrogen bonding (H positive)
- Mixed (graphite)

Crystal dynamics, phonons (Ch 2)

- Quantum vibrations ,T=0
- Temperature vibrations T>0

Sound waves

$$\omega = \mathrm{v}\, k$$

Three types of sound waves: one *longitudinal* +
two *transverse*

Velocity

$\zeta(x)$ – displacement.

Compare $\zeta(\mathrm{x})$ and $\zeta(\mathrm{x}+\delta\mathrm{x})=\zeta(\mathrm{x})+\delta\mathrm{x}\dfrac{\partial\zeta(x)}{\partial\mathrm{x}}$.

Extension of $\delta\mathrm{x}$ is $\delta x\dfrac{\partial\zeta}{\partial\mathrm{x}}$.

$$\text{Strain} = \frac{\partial\zeta}{\partial\mathrm{x}}$$

Hook law: strain proportional to stress (force per area)

$$\Gamma = C\frac{\partial\zeta}{\partial x}, \quad C - \text{elastic modulus}$$

Velocity, Hook's and Newton's laws

Hook's law $\Gamma = C \dfrac{\partial \zeta}{\partial x}$

Newton's law $\Gamma(x + \delta x) - \Gamma(x) = \delta x \dfrac{\partial \Gamma}{\partial x} = \delta m \dfrac{\partial^2 \zeta}{\partial t^2}$

$$\delta\mu = \rho \delta x$$

$$C \frac{\partial^2 \zeta}{\partial x^2} = \rho \frac{\partial^2 \zeta}{\partial t^2}$$

$$\frac{\partial^2 \zeta}{\partial x^2} = \frac{1}{\mathrm{v}_L{}^2} \frac{\partial^2 \zeta}{\partial t^2}$$

$$\mathrm{v}_L = \sqrt{\frac{C}{\rho}} \qquad (C \rightarrow E = \rho \mathrm{v}_L{}^2)$$