



Lecture 17

Waves in and into/out-of Crystal

Crystal Translation Symmetry and
Bloch's theorem

Crystal Momentum Conservation

- $\mathbf{k}_f - \mathbf{k}_i = \mathbf{G}$ for Bragg Scattering
- This can be generalized for inelastic processes to (Bloch's theorem)

$$\mathbf{k}_f - \mathbf{k}_i - \mathbf{q}_e = \mathbf{G}$$

which holds for inelastic scattering for all experiments involving waves (electron, neutron, photon ...) or any scattering processes that occur inside the crystal.

- Combining with the energy conservation rule, dispersion relations of phonons, electrons, spin waves etc. are routinely measured by neutron, photon, electrons as probes.

Neutron Scattering of Phonons

- 0 phonon scattering: neutron init $\mathbf{p} = \hbar\mathbf{q}$, neutron final $\mathbf{p}' = \hbar\mathbf{q}'$, $q' = q$, $\mathbf{q}' = \mathbf{q} + \mathbf{K}$.
- 1 phonon scattering:

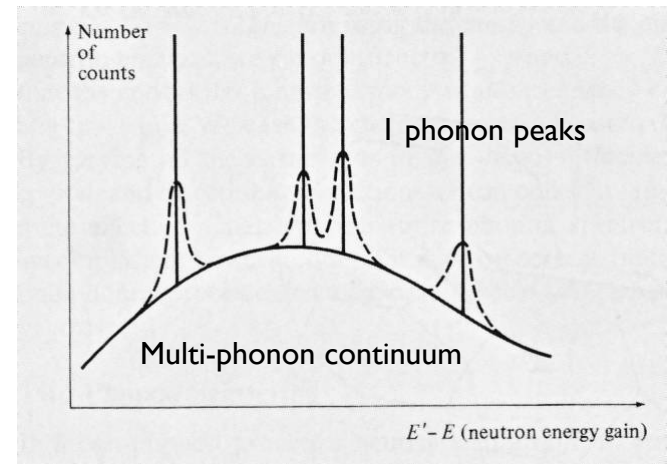
$$\begin{aligned}
 E' &= E + \hbar\omega_s(\mathbf{k}), & \frac{p'^2}{2M_n} &= \frac{p^2}{2M_n} + \hbar\omega_s\left(\frac{\mathbf{p}' - \mathbf{p}}{\hbar}\right), & \text{phonon absorbed,} \\
 \mathbf{p}' &= \mathbf{p} + \hbar\mathbf{k} + \hbar\mathbf{K}, \\
 E' &= E - \hbar\omega_s(\mathbf{k}), & \frac{p'^2}{2M_n} &= \frac{p^2}{2M_n} - \hbar\omega_s\left(\frac{\mathbf{p} - \mathbf{p}'}{\hbar}\right), & \text{phonon emitted.} \\
 \mathbf{p}' &= \mathbf{p} - \hbar\mathbf{k} + \hbar\mathbf{K},
 \end{aligned}$$

- Multi-phonon scattering

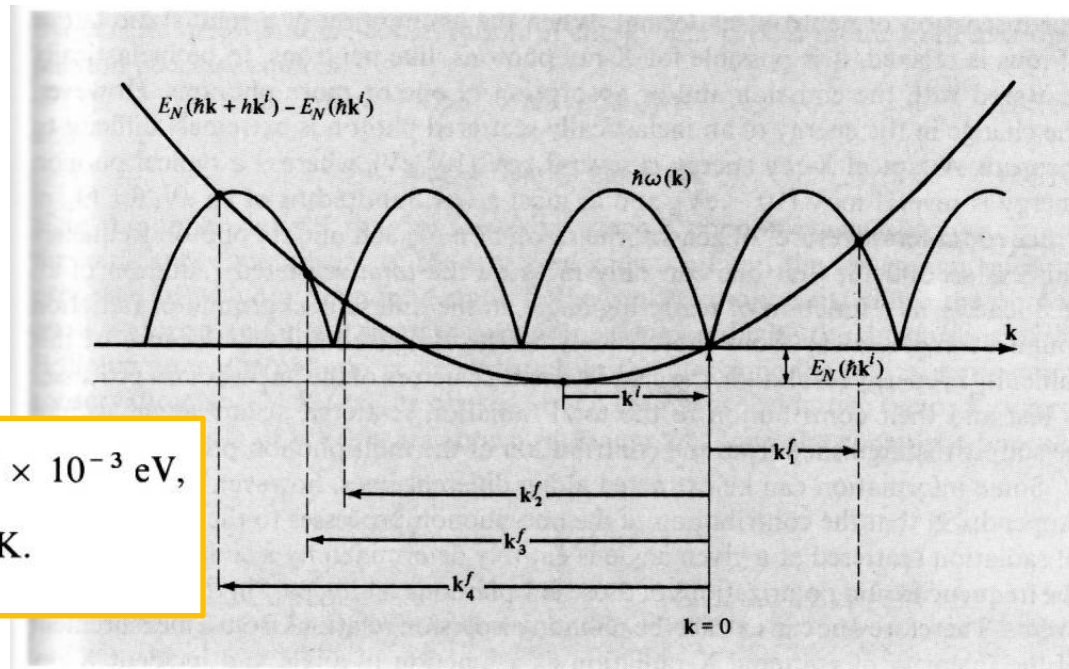
$$\begin{aligned}
 E' &= E + \hbar\omega_s(\mathbf{k}) + \hbar\omega_s(\mathbf{k}'), \\
 \mathbf{p}' &= \mathbf{p} + \hbar\mathbf{k} + \hbar\mathbf{k}' + \hbar\mathbf{K}.
 \end{aligned}$$

2 phonon absorption

$$E' = E + \hbar\omega_s(\mathbf{k}) + \hbar\omega_{s'}\left(\frac{\mathbf{p}' - \mathbf{p}}{\hbar} - \mathbf{k}\right).$$



Energy, momentum conservation



$$E_N = 2.1(q[\text{\AA}^{-1}])^2 \times 10^{-3} \text{ eV},$$

$$\frac{E_N}{k_B} = 24(q[\text{\AA}^{-1}])^2 \text{ K}.$$

Figure 24.6

Graphical solution to the one-phonon conservation laws when the incident neutron has wave vector \mathbf{k}^i . The conservation law for phonon absorption can be written

$$E_N(\hbar\mathbf{k} + \hbar\mathbf{k}^i) - E_N(\hbar\mathbf{k}^i) = \hbar\omega(\mathbf{k}),$$

where $\hbar\mathbf{k}$ is the momentum of the scattered neutron, and $E_N(\mathbf{p}) = p^2/2M_N$. To draw the left-hand side of this equation, one displaces the neutron energy-momentum curve horizontally so that it is centered at $\mathbf{k} = -\mathbf{k}^i$ rather than $\mathbf{k} = 0$, and displaces it downward by an amount $E_N(\hbar\mathbf{k}^i)$. Solutions occur wherever this displaced curve intersects the phonon dispersion curve $\hbar\omega(\mathbf{k})$. In the present case there are solutions for four different scattered neutron wave vectors, $\mathbf{k}_1^f \cdots \mathbf{k}_4^f$.

Optical or X-Ray Measurement

$$\hbar\omega' = \hbar\omega \pm \hbar\omega_s(\mathbf{k})$$

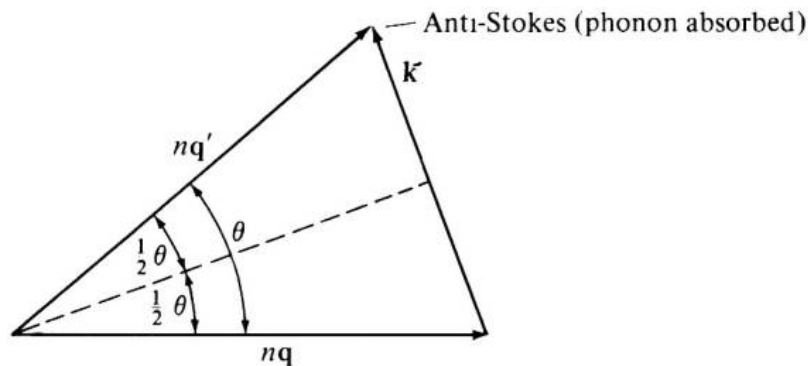
Optical Phonons – Raman Scattering
Acoustic Phonons – Brillouin Scattering

$$\hbar n\mathbf{q}' = \hbar n\mathbf{q} \pm \hbar\mathbf{k} + \hbar\mathbf{K}$$

Laser light is used (\sim a few 1000 Å wavelength with \sim eV E)

$$|\mathbf{q}'| \approx |\mathbf{q}|$$

$\mathbf{k} \sim 0$ is probed



Raman, Brillouin

$$k = 2nq \sin \frac{1}{2}\theta = (2\omega n/c) \sin \frac{1}{2}\theta.$$

Brillouin

$$c_s(\hat{\mathbf{k}}) = \frac{\Delta\omega}{2\omega} \frac{c}{n} (\csc \frac{1}{2}\theta).$$

It is also possible to probe phonons using High energy X-ray (10 keV) using modern synchrotrons (such as ESRF, APS).