Dr. Gregory W. Clark
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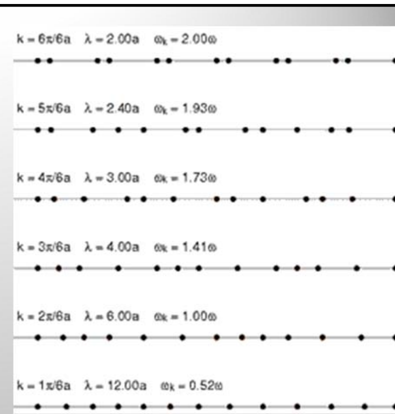
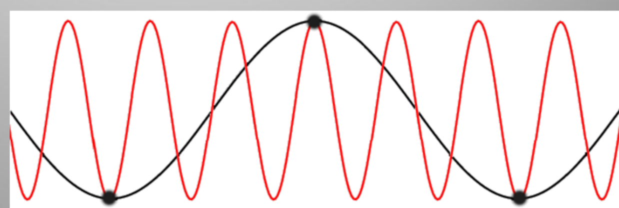




PHYS432
Materials Physics

Pop Quiz

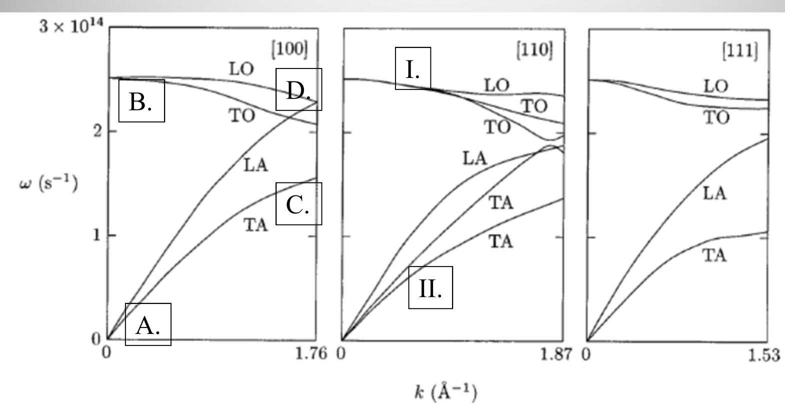
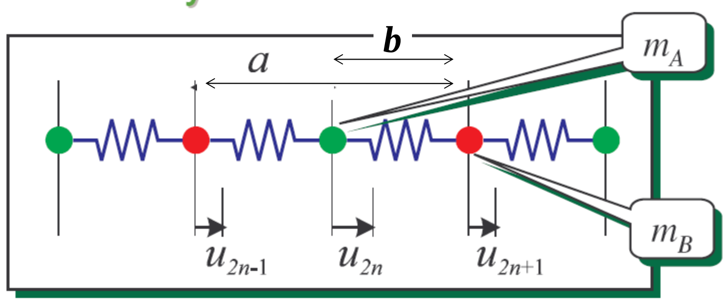


Fig. 3-24. Dispersion curves for diamond (C) in the first Brillouin zone. Data are from J. L. Warren, G. Dolling, and R. A. Cowley, *Phys. Rev.* **158**, 805 (1967).

Diatomic Lattice

- Now try two different masses connected by same strength "spring" bonds

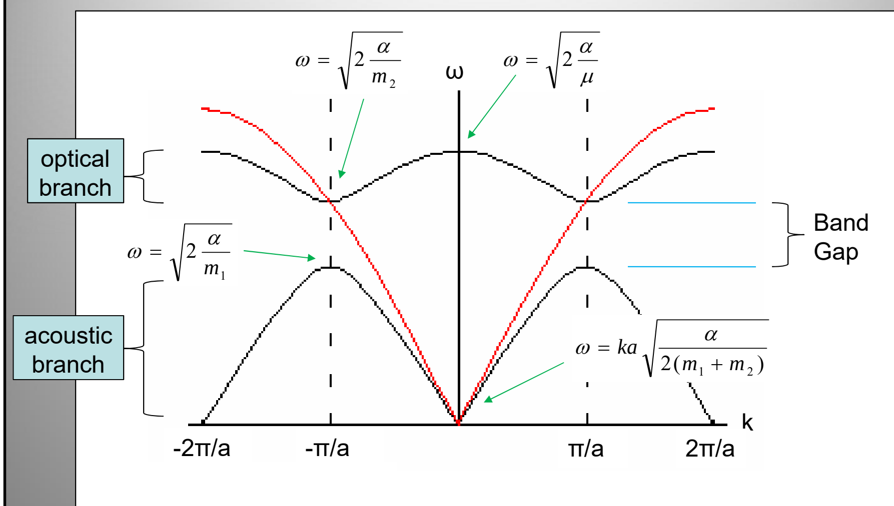
Technically a lattice with a basis



Dispersion relation: $$\omega^2 = \alpha\left(\frac{1}{m_A}+\frac{1}{m_B}\right) \pm \alpha\sqrt{\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^2 - \frac{4\sin^2(ka/2)}{m_A m_B}}$$

Dispersion plot

Diatomic Lattice

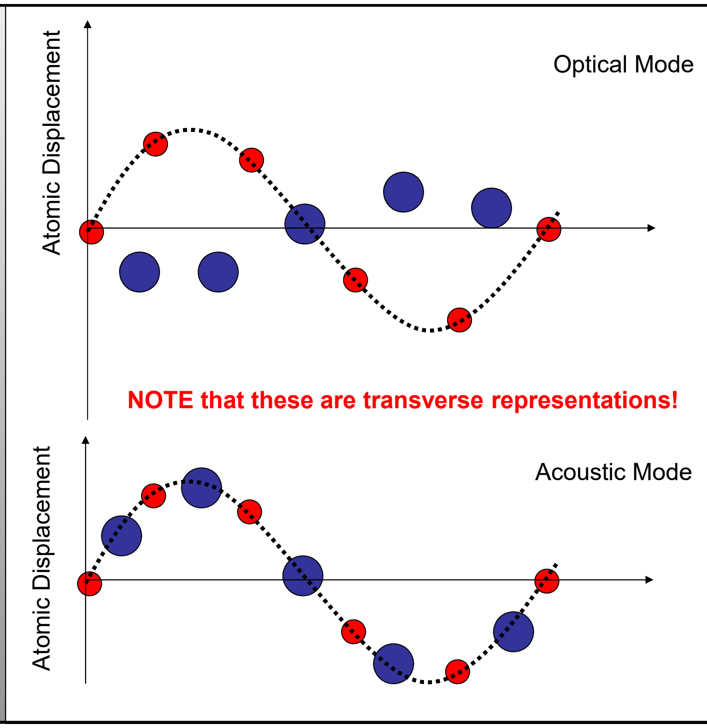


$$\left.\frac{A_2}{A_1}\right|_{k=0} = -\frac{m_1}{m_2}$$

Stokes' models

Animations

$$\left.\frac{A_2}{A_1}\right|_{k\to 0} = 1$$



Diatomic Lattice

Acoustic modes:

- Correspond to sound-waves in the long- λ limit.
- ω→0 as k → *0*

Optical modes:

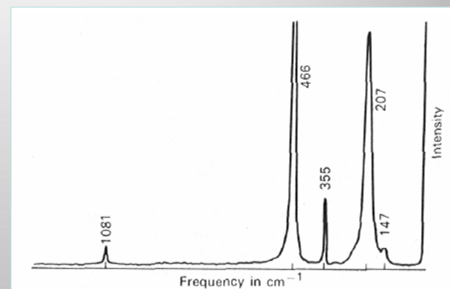
- In the long-λ limit, optical modes interact strongly with electromagnetic radiation in polar crystals.
- Strong optical absorption is observed (photons annihilated, phonons created; often in IR part of spectrum).
- w → finite value as k → *0*
- Optical modes arise from folding back the dispersion curve as the lattice periodicity is doubled (halved in k-*space).*

Zone boundary:

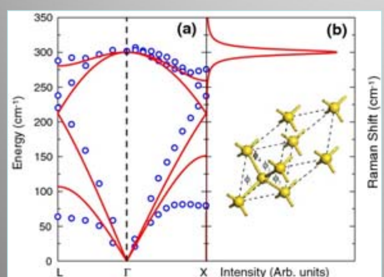
- All modes are standing waves at zone boundary, ∂ω / ∂k = *0:* a necessary consequence of the lattice periodicity.
- In a diatomic chain, the frequency-gap between the acoustic and optical branches depends on the mass difference. In the limit of identical masses the gap → zero.

e.g., exciting optical modes

- Raman scattering:
- near-IR, vis, near-UV



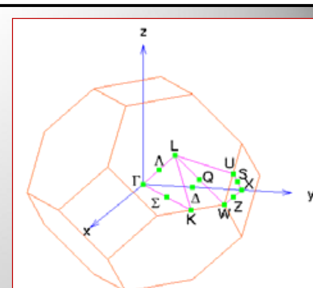
Scattered light has peaks at $h\nu = h\nu_o \pm \hbar\omega_{phonon}$



Raman response of c-Ge

Must extrapolate these results to 3D

- Dispersion curves for Cu
- Note that transverse waves are now possible



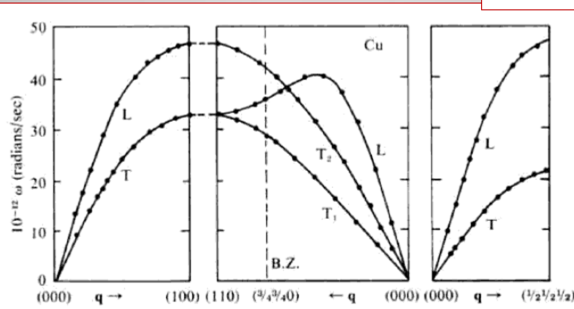
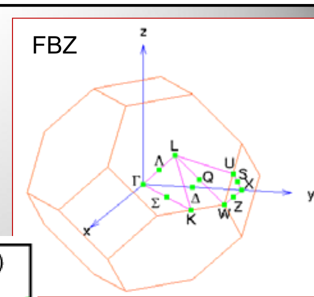
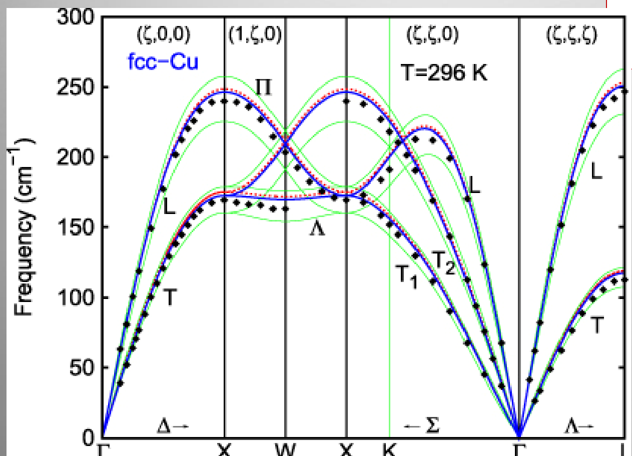


Fig. 24.6 The phonon dispersion in copper (Cu). Because Cu is a three-dimensional metal, the phonon dispersion has to be evaluated in three dimensions, and it is here shown as a function of wave vector in different directions. Along the (101) direction, bands can be seen which look somewhat like the simple monatomic chain. Both longitudinal (L) and transverse (T) modes are present. The wave vector q is plotted in units of π/a where a is the lattice spacing. The data shown are from Svensson et al., Phys. Rev. B **155**, 619 (1967), and are obtained using inelastic neutron scattering. In this technique, a beam of slow neutrons is scattered from the sample and the changes in both the energy and momentum of the neutrons are measured.

Must extrapolate these results to 3D

- Dispersion curves for Cu
- Points are experimental data

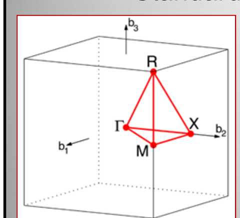


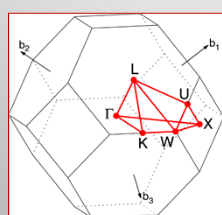


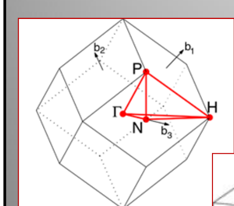
All acoustic for Cu!

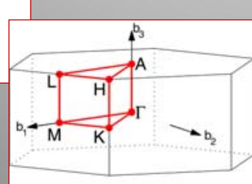
- Critical points

Standard notation!









Symbol	Description
Γ	Center of the Brillouin zone
	Simple cube
M	Center of an edge
R	Corner point
X	Center of a face
	Face-centered cubic
K	Middle of an edge joining two hexagonal faces
L	Center of a hexagonal face
U	Middle of an edge joining a hexagonal and a square face
W	Corner point
X	Center of a square face
	Body-centered cubic
H	Corner point joining four edges
N	Center of a face
P	Corner point joining three edges
	Hexagonal
A	Center of a hexagonal face
H	Corner point
K	Middle of an edge joining two rectangular faces
L	Middle of an edge joining a hexagonal and a rectangular face
M	Center of a rectangular face

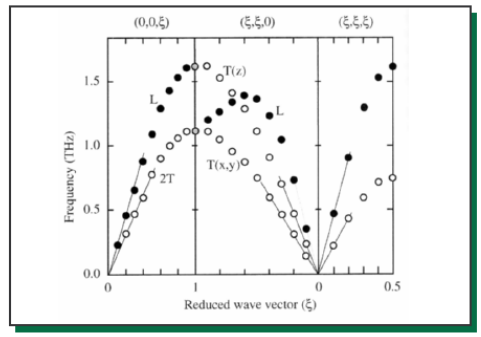
https://en.wikipedia.org/wiki/Brillouin_zone

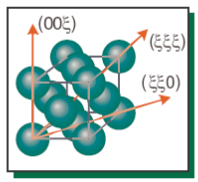
❖Monatomic Example: Neon, a FCC solid below 24.6K

➢ Inelastic neutron scattering results in different crystallographic directions

Many features fit 1-D model:

- Dispersion is sinusoidal (n.n. interactions)
- All modes are acoustic (monatomic system)
- Two distinct modes:
  Longitudinal (L), (generally higher energy)
  Transverse (T), (often degenerate)





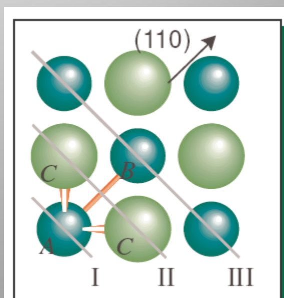
Phys. Rev. *B* **11**, 1681, (1975)

❖Monatomic Example: Neon, a FCC solid below 24.6K

Minor point (*demonstrating that real systems are subtle and interesting, but also complicated!*):

L mode along (ξ ξ 0) has 2 Fourier components, suggesting next-nearest neighbor interactions. In fact there are only nearest neighbor interactions! The effect is due to the FCC structure.

For atom A, atoms C and B are nearest-neighbors, but in different planes (II and III)!

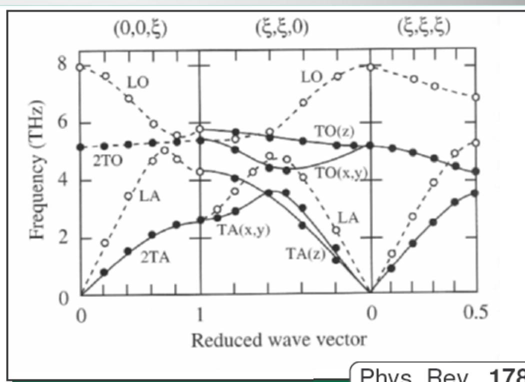


❖Diatomic Example: NaCl, a FCC solid

- ➢ Can visualize as two interpenetrating FCC lattices

The 1-D model gives several insights:

- Optical and acoustic modes (labels O and A);
- Longitudinal and transverse modes (L and T).
- Dispersion along (ξ ξ ξ) is simplest and most like our 1-D model
- (ξ ξ ξ) planes contain, alternately, Na atoms and Cl atoms (other directions have Na and Cl mixed)



Phys. Rev. **178** 1496, (1969)

NOTE higher E's than with Ne – stronger bonding!

Phonon Dispersion for KBr

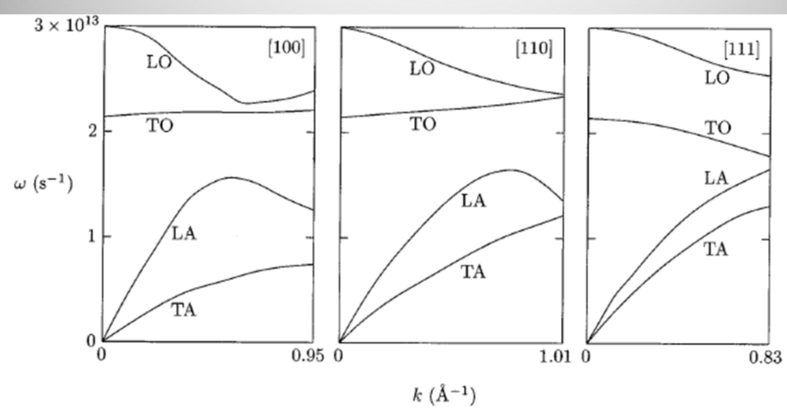


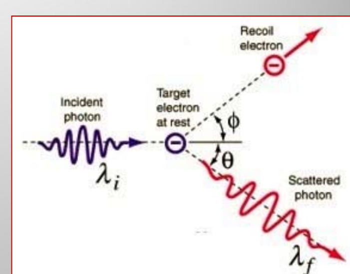
Fig. 3-23. Dispersion curves in potassium bromide (KBr) in the first Brillouin zone. Data are from A. D. B. Woods, B. N. Brockhouse, and R. A. Cowley, *Phys. Rev.* **131**, 1025 (1963).

How do we determine these lattice wave (phonon) dispersion relations experimentally?

- *Phonon scattering of neutrons or photons!*
- *To get a sense for this, we need to examine scattering from a quantum mechanical perspective …*

Photon scattering by electrons (Compton effect)

- Arthur Compton, 1923
- 1927 Nobel Prize
- Light behaves like a particle!
- Inelastic scattering of photons by the e^- in atoms
- Photons are quanta of E

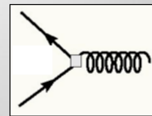


E conservation: $\hbar\omega_i = \hbar\omega_f + E_e$

$\vec{p}$ conservation: $\hbar\vec{k}_i = \hbar\vec{k}_f + \vec{p}_e$

Neutron scattering by phonons

- Inelastic scattering of neutrons
- Phonons are quanta of E



	Phonon emission	Phonon adsorption
E conservation:	$E_f = E_i - \hbar\omega$	$E_f = E_i + \hbar\omega$
$\vec{p}$ conservation:	$\vec{p}_f = \vec{p}_i - \hbar\vec{k}$	$\vec{p}_f = \vec{p}_i + \hbar\vec{k}$

"crystal momentum"

Note: *phonon wavevector not uniquely determined – can have any value that satisfies* $\vec{k}' = \vec{G} + \vec{k}$ *, so can always map back into FBZ and describe the same wave!*