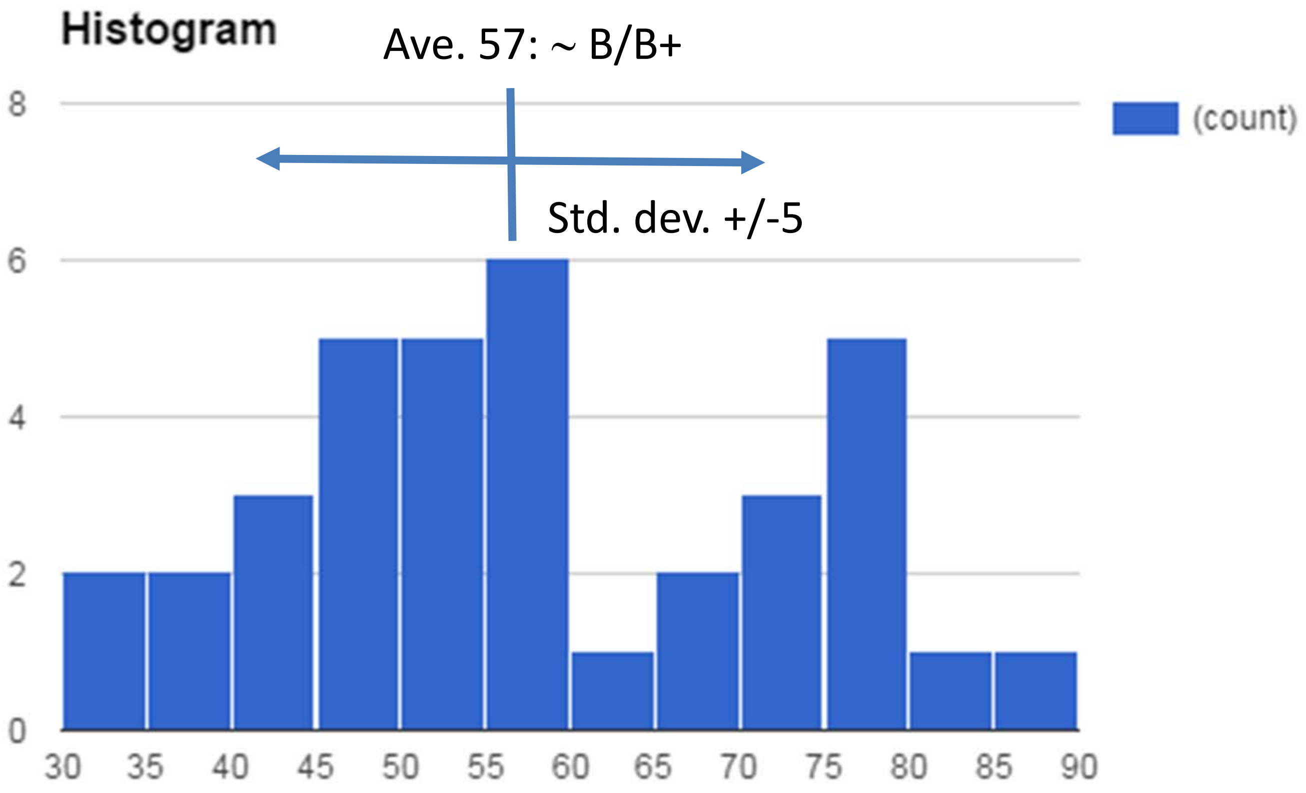
Midterm grades



Ave. 57: ~ B/B+

Std. dev. +/-5

Physics 140A-Introduction to Solid State Physics
Winter, 2016
Problem Set 3
Due Thursday, 18 February

Reading: Finish Omar, Chapter 2, Read Chapter 3 on Lattice Vibrations, Sections 3.1-3.10

Plus supplemental reading from Kittel on Debye-Waller factors

Diffraction:

(Questions and Problems in Omar from Chapter 2 indicated as 2.x)

[1] Question 2.1
[2] Question 2.2 (We discussed this in lecture.)
[3] Question 2.3
[4] Problem 2.3.
[5] Problem 2.6. A hint here is to let the vector s lie along the z direction in spherical polar coordinates, which simplifies the integration greatly.
[6] Problem 2.8 (Also discussed in lecture in more detail.)
[7] Problem 2.9. Hint: You can let the limit on the integral R go to infinity, since the hydrogen wave function dies off quickly in r due to the exponential in its charge density.
[8] Problem 2.13
[9] Problem 2.19, plus as an additional part show the <u>Ewald construction</u> for diffraction of 10.0 keV x-rays incident on this 2D crystal along the direction of the basis vector $\vec{a}$, and comment on whether any diffraction spots would be observed.
[10] Problem 2.20,
  (d) Reword as: A general formula for the Bragg angle for reflection from the above (210) planes.
  Plus additional special part as:
  (e) Show with one or more cross-sections and/or 3D sketches what the <u>first Brillouin zone</u> would look like for this unit cell.
[11] Problem 2.25

Physics 140A-Introduction to Solid State Physics
Winter, 2016
Problem Set 4 (One shorter one to go after this)
Due Tuesday, March 1st

Lattice Vibrations: Thermal and Acoustic Properties

Reading: Omar, Sections 3.1 through 3.10 (only thorough Inelastic X-ray Scattering, plus two pages on thermal conductivity from Kittel as Supplemental Reading.

Questions and Problems in Omar from Chapter 3.

[1] Question 3.1

[2] Question 3.4

[3] Problem 3.2

[4] Problem 3.5

[5] Problem 3.6

[6] Problem 3.10

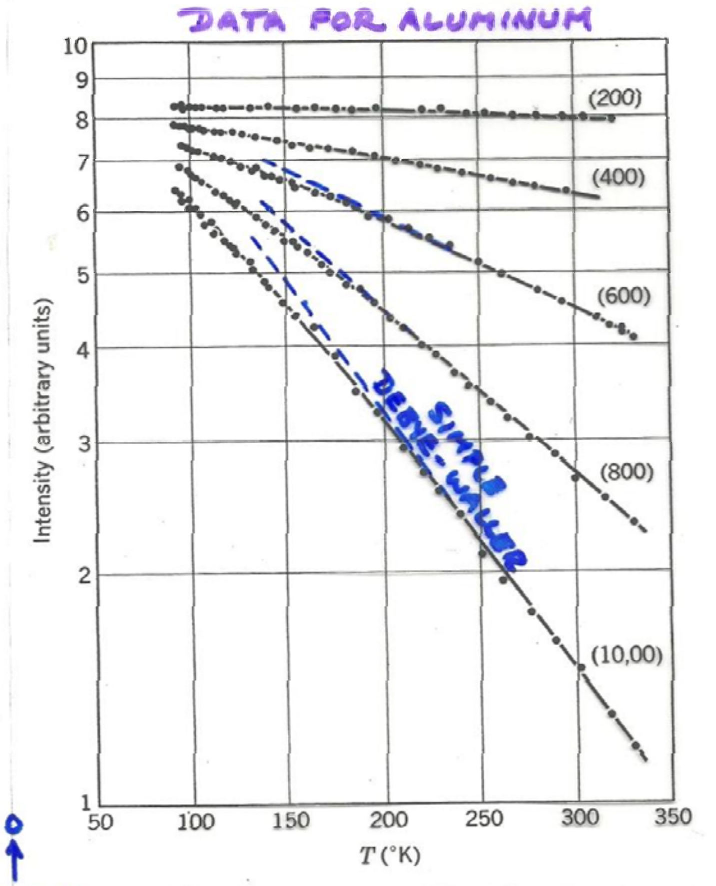
[7] Problem 3.19

[8] Special: Derive Eq. 2.26 from the two equations preceding it

[9] Special: Derive Eqs. 3.50 and 3.51 from 3.44

Back to solids: Vibrational effects on diffraction: the Debye-Waller factor

Vibrations smear positions, decrease diffraction→phonons



See supplementary reading from Kittel on Debye-Waller factor

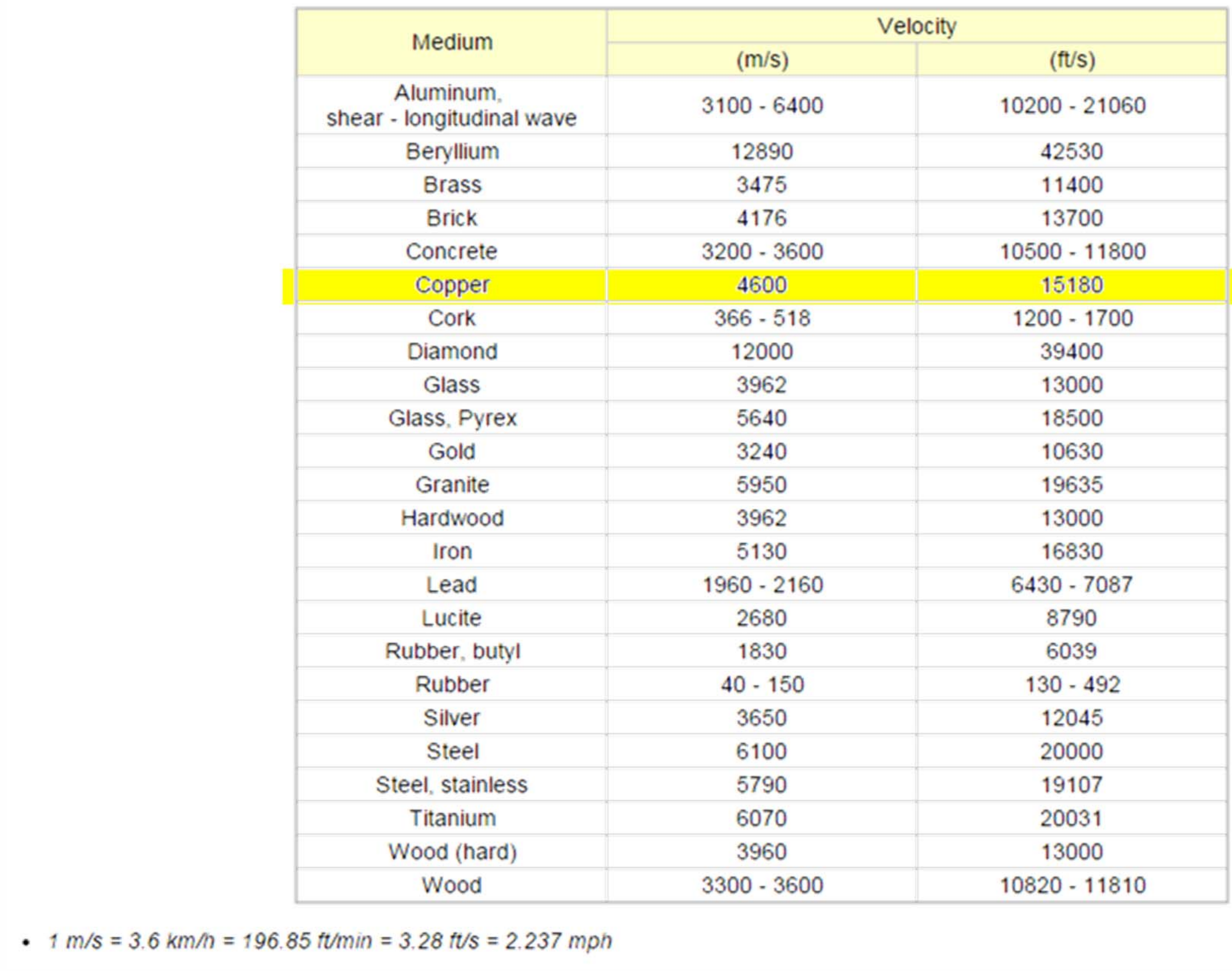
0
↑
RESIDUAL ZERO-POINT VIBRATION

$$I_{hk\ell}(T) = I_{hk\ell}(\text{rigid lattice})\exp\left[-\frac{1}{3}\langle u^2\rangle G_{hk\ell}^2\right],$$

if harmonic oscillator with mass M and frequency $\omega = \sqrt{\frac{k}{M}}$,

$$= I_{hk\ell}(\text{rigid lattice})\exp\left[\frac{-k_B T G_{hk\ell}^2}{M\omega^2}\right]$$

Speed of sound in various materials



Medium	Velocity	
	(m/s)	(ft/s)
Aluminum, shear - longitudinal wave	3100 - 6400	10200 - 21060
Beryllium	12890	42530
Brass	3475	11400
Brick	4176	13700
Concrete	3200 - 3600	10500 - 11800
Copper	4600	15180
Cork	366 - 518	1200 - 1700
Diamond	12000	39400
Glass	3962	13000
Glass, Pyrex	5640	18500
Gold	3240	10630
Granite	5950	19635
Hardwood	3962	13000
Iron	5130	16830
Lead	1960 - 2160	6430 - 7087
Lucite	2680	8790
Rubber, butyl	1830	6039
Rubber	40 - 150	130 - 492
Silver	3650	12045
Steel	6100	20000
Steel, stainless	5790	19107
Titanium	6070	20031
Wood (hard)	3960	13000
Wood	3300 - 3600	10820 - 11810

- *1 m/s = 3.6 km/h = 196.85 ft/min = 3.28 ft/s = 2.237 mph*

15180 ft/s
≈ 3 miles/s

For copper:
Y = 120
120 x 10^9 nt/m^2;
density = 8,940 kg/m^3
Gives
Sqrt[Y/ρ] = 3663 m/s

Summing over vibrational modes in 1D and 3D

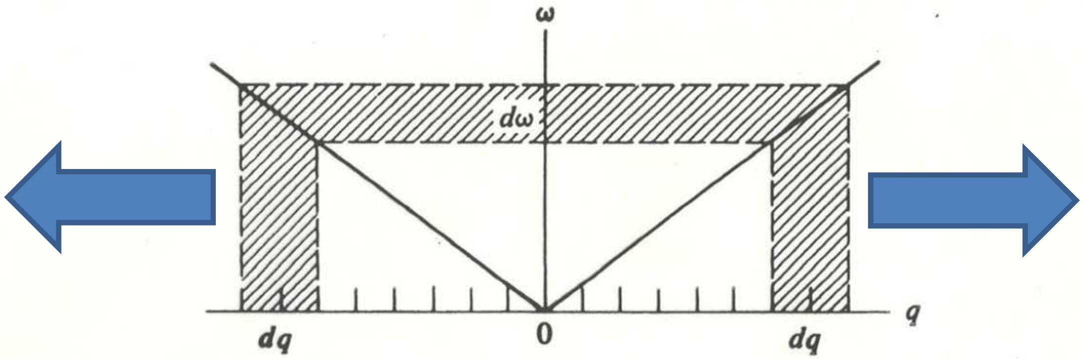
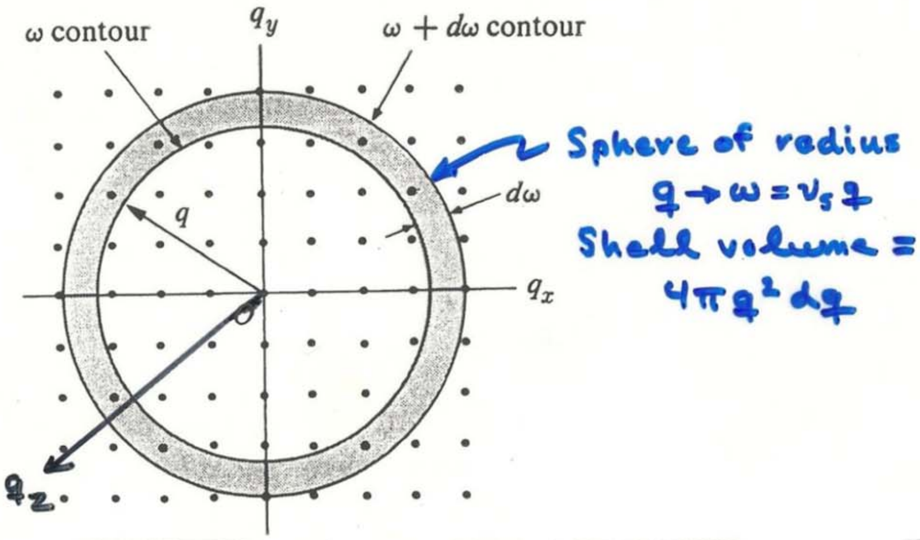


Fig. 3.4 The enumeration of modes. The dispersion curve is composed of two segments: $\omega = v_s q$ and $\omega = -v_s q$. The former represents waves traveling to the right, the latter waves traveling to the left.



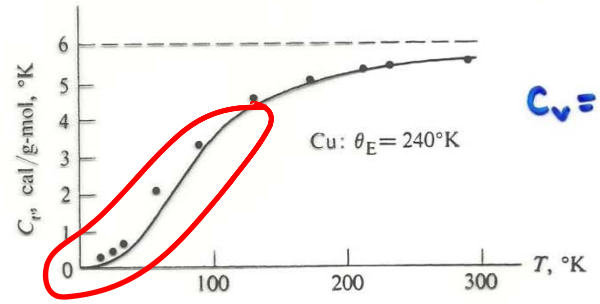
Sphere of radius $q \rightarrow \omega = v_s q$

Shell volume = $4\pi q^2 dq$

Fig. 3.5 Allowed values of **q** for a wave traveling in 3 dimensions. (Only the cross section in the $q_x q_y$-plane is shown.) The shaded circular shell is used for counting the modes.

Vibrational effects on heat capacities: Einstein and Debye models

EINSTEIN: INDEPENDENT HARMONIC OSCILLATORS - QUANTIZED, $\varepsilon_n = n\hbar\omega_n$



$$C_v = 3R\left(\frac{\theta_E}{T}\right)^2 \cdot \frac{e^{\theta_E/T}}{\left(e^{\theta_E/T} - 1\right)^2}$$

Fig. 3.10 Specific heat of copper versus temperature. The dots represent experimental values, and the curve is given by the Einstein expression.

The Debye model for phonon statistics: Cutoff to yield $3N_A$ modes/mole

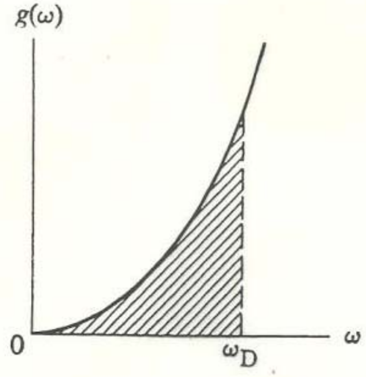


Fig. 3.11 The Debye cutoff procedure. The shaded area is equal to the number of modes which is $3N_A$.

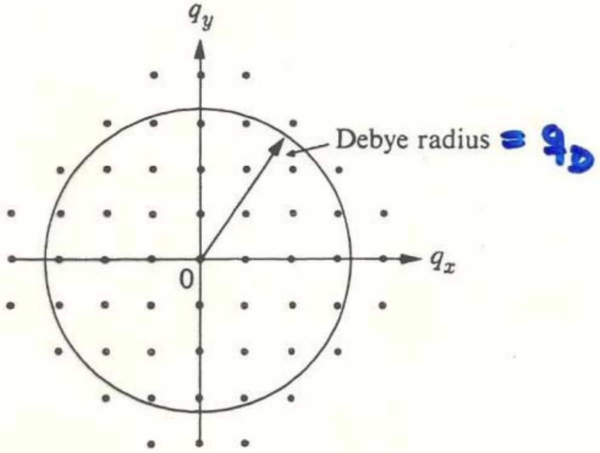
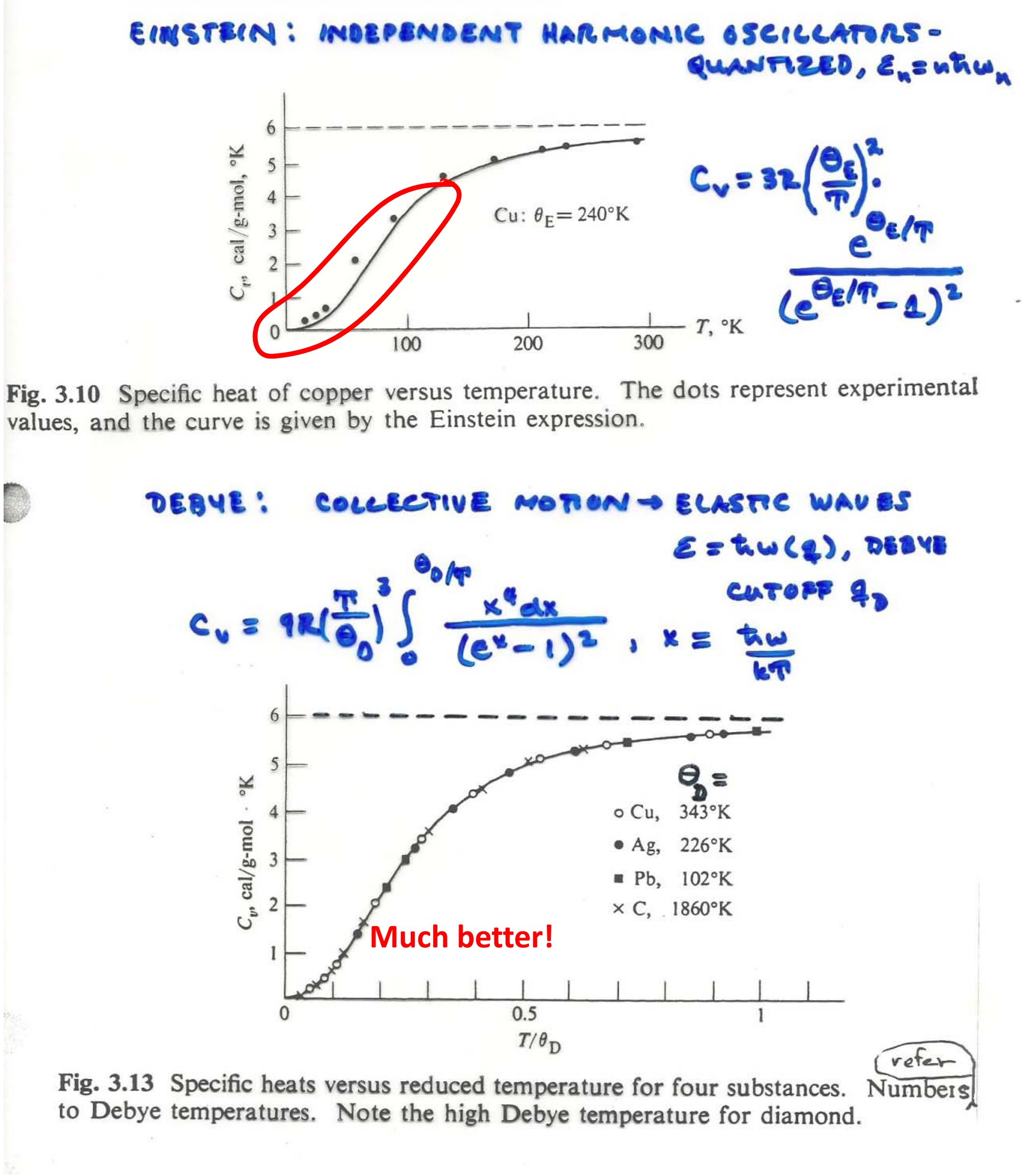


Fig. 3.12 The Debye sphere.

Vibrational effects on heat capacities: Einstein and Debye models



EINSTEIN: INDEPENDENT HARMONIC OSCILLATORS - QUANTIZED, $\varepsilon_n = n\hbar\omega_n$

$$C_v = 3R\left(\frac{\Theta_E}{T}\right)^2 \cdot \frac{e^{\Theta_E/T}}{(e^{\Theta_E/T}-1)^2}$$

Fig. 3.10 Specific heat of copper versus temperature. The dots represent experimental values, and the curve is given by the Einstein expression.

DEBYE: COLLECTIVE MOTION → ELASTIC WAVES

$\varepsilon = \hbar\omega(q)$, DEBYE CUTOFF q_D

$$C_v = 9R\left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4\,dx}{(e^x-1)^2}, \quad x = \frac{\hbar\omega}{kT}$$

Fig. 3.13 Specific heats versus reduced temperature for four substances. Numbers refer to Debye temperatures. Note the high Debye temperature for diamond.

Low temperature heat capacity of solid argon and the Debye model: no electronic contribution

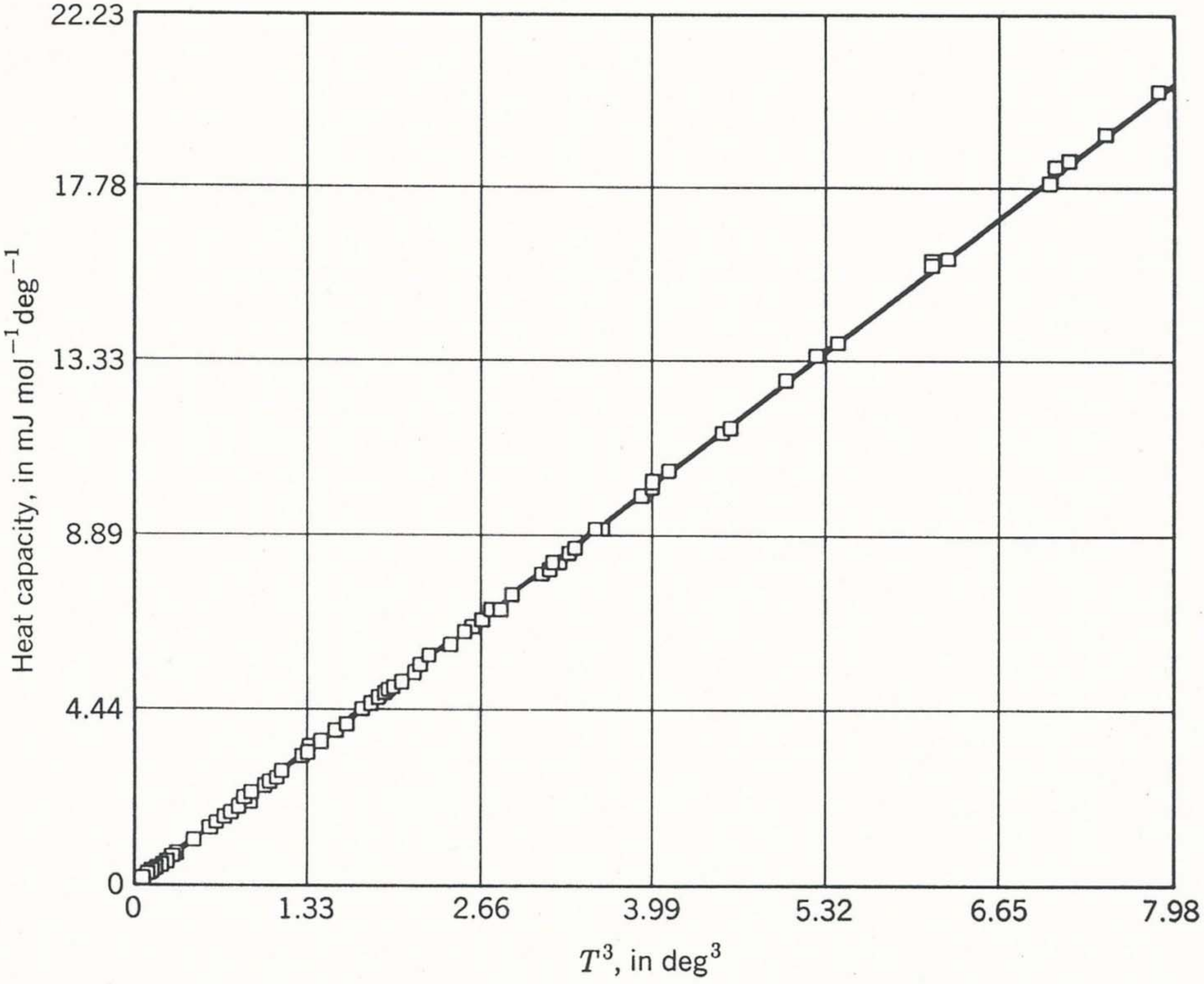


Figure 16 Low temperature heat capacity of solid argon, plotted against T^3. In this temperature region the experimental results are in excellent agreement with the Debye T^3 law with $\theta_0 = 92.0$ deg. (Courtesy of L. Finegold and N. E. Phillips.)

Debye temperatures of some materials

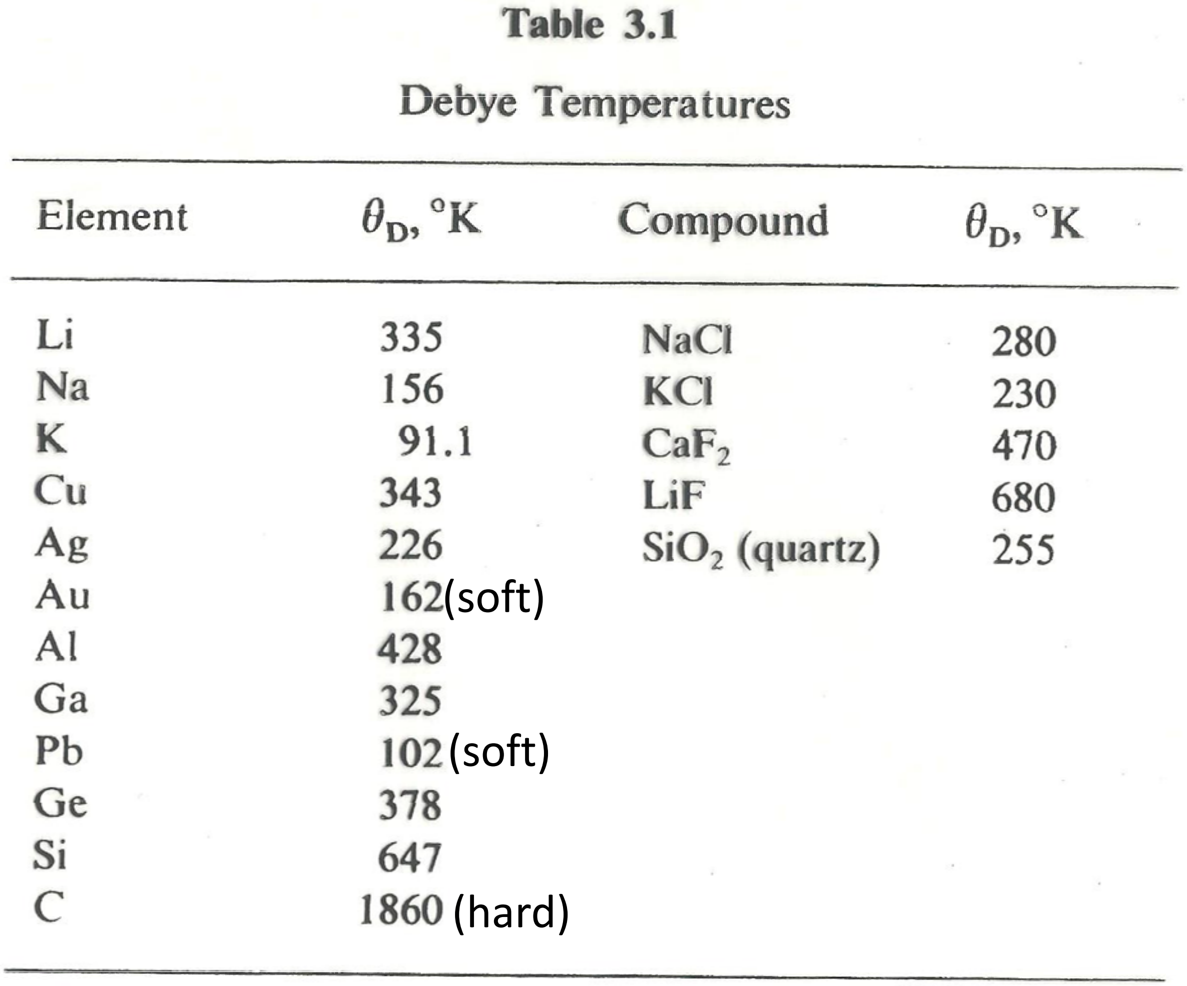
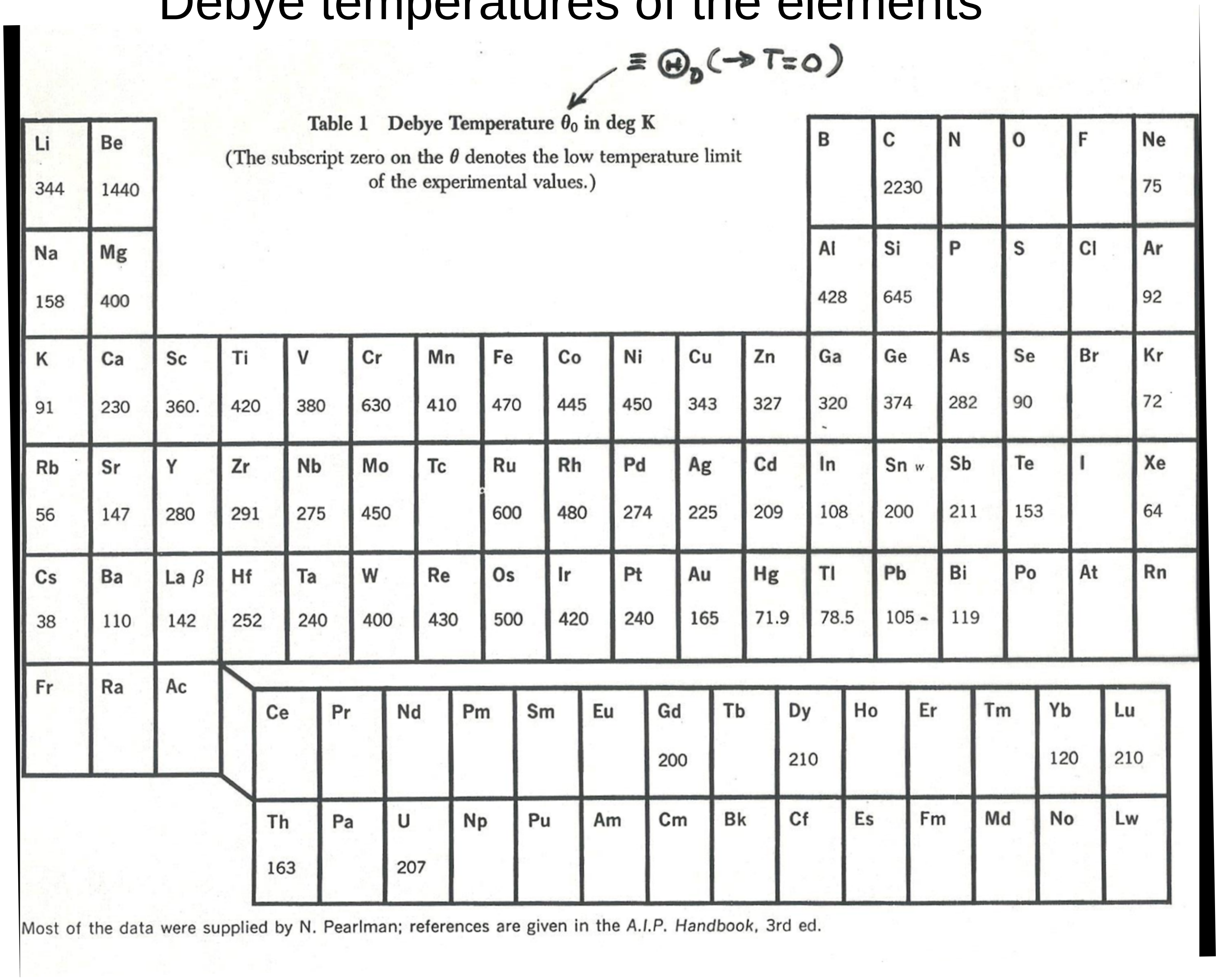


Table 3.1

Debye Temperatures

Element	θ_D, °K	Compound	θ_D, °K
Li	335	NaCl	280
Na	156	KCl	230
K	91.1	CaF_2	470
Cu	343	LiF	680
Ag	226	SiO_2 (quartz)	255
Au	162(soft)		
Al	428		
Ga	325		
Pb	102 (soft)		
Ge	378		
Si	647		
C	1860 (hard)		

Debye temperatures of the elements



$\equiv \Theta_D (\to T=0)$

Table 1 Debye Temperature θ_0 in deg K

(The subscript zero on the θ denotes the low temperature limit of the experimental values.)

Li 344	Be 1440											B	C 2230	N	O	F	Ne 75
Na 158	Mg 400											Al 428	Si 645	P	S	Cl	Ar 92
K 91	Ca 230	Sc 360.	Ti 420	V 380	Cr 630	Mn 410	Fe 470	Co 445	Ni 450	Cu 343	Zn 327	Ga 320	Ge 374	As 282	Se 90	Br	Kr 72
Rb 56	Sr 147	Y 280	Zr 291	Nb 275	Mo 450	Tc	Ru 600	Rh 480	Pd 274	Ag 225	Cd 209	In 108	Sn *w* 200	Sb 211	Te 153	I	Xe 64
Cs 38	Ba 110	La β 142	Hf 252	Ta 240	W 400	Re 430	Os 500	Ir 420	Pt 240	Au 165	Hg 71.9	Tl 78.5	Pb 105	Bi 119	Po	At	Rn
Fr	Ra	Ac															

Ce	Pr	Nd	Pm	Sm	Eu	Gd 200	Tb	Dy 210	Ho	Er	Tm	Yb 120	Lu 210
Th 163	Pa	U 207	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

Most of the data were supplied by N. Pearlman; references are given in the *A.I.P. Handbook*, 3rd ed.

Energies of 1D vibrational waves as a function of wavevector q

$v_g = \omega/dq = 0$

Standing wave

Continuum model:

$\omega = \mathrm{sqrt}[Y/\rho]q$, $v_s = \mathrm{sqrt}[Y/\rho]$

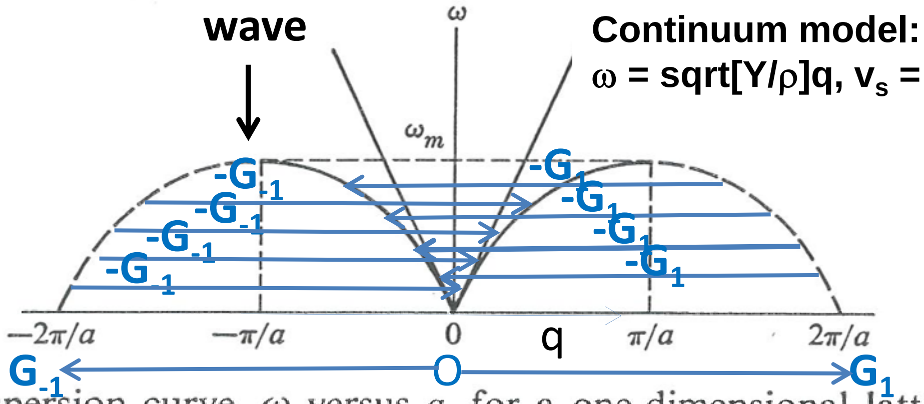
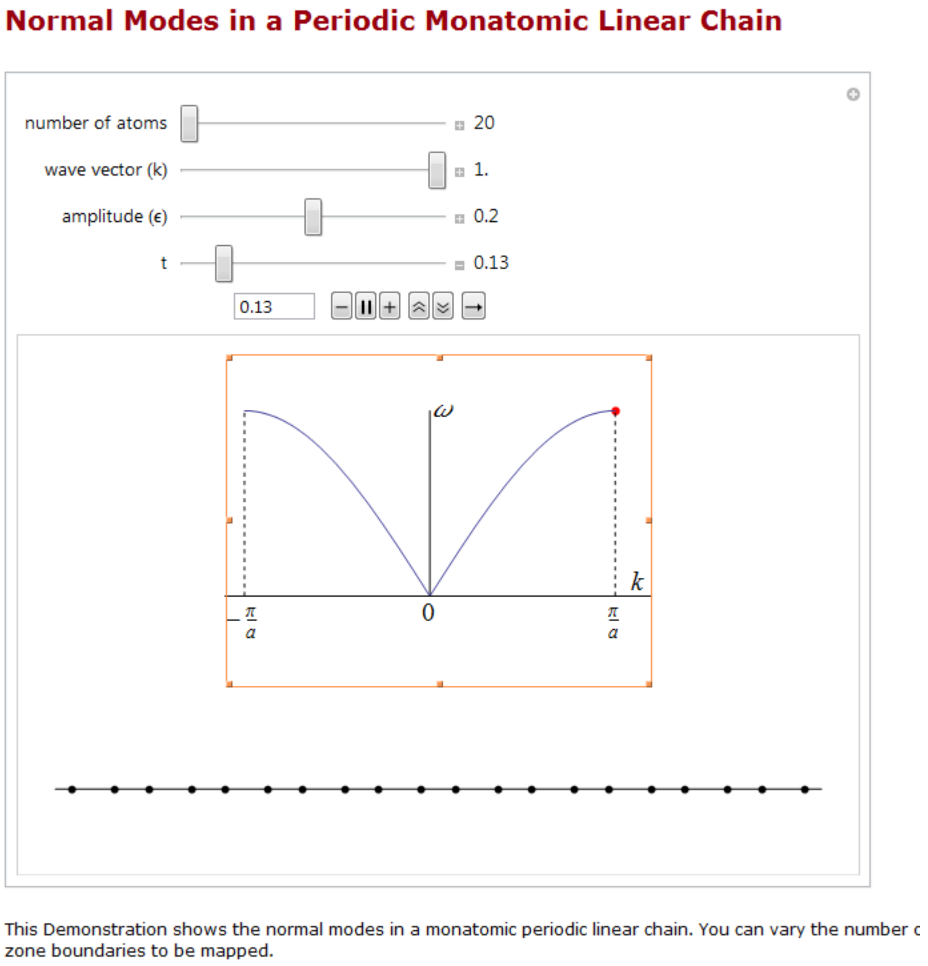


Fig. 3.17 The dispersion curve, ω versus q, for a one-dimensional lattice with nearest-neighbor interaction. The curve is periodic, but is drawn as a dashed line outside the region $-\pi/a < q < \pi/a$ (see text).

Playtime with the monatomic linear chain
(In 3D, like primitive lattice with one atom/cell: e.g. fcc and bcc, no optical modes)



Normal Modes in a Periodic Monatomic Linear Chain

number of atoms 20

wave vector (k) 1.

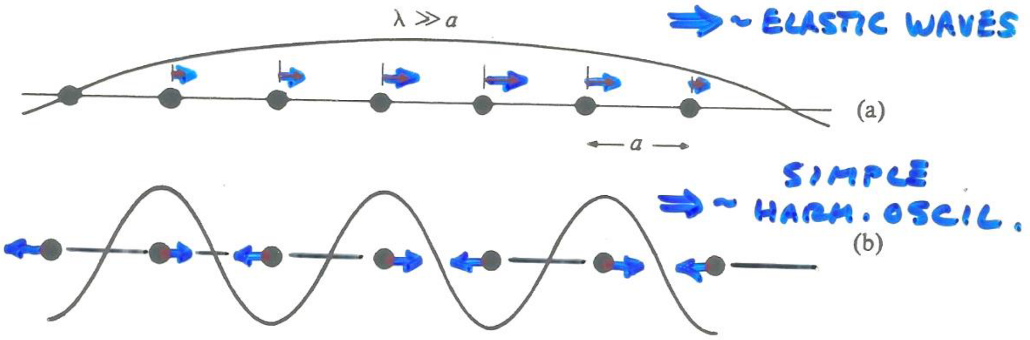
amplitude (ϵ) 0.2

t 0.13

This Demonstration shows the normal modes in a monatomic periodic linear chain. You can vary the number c
zone boundaries to be mapped.

http://demonstrations.wolfram.com/NormalModesInAPeriodicMonatomicLinearChain/

Basics of vibrational waves on a lattice



⇒ ~ ELASTIC WAVES

SIMPLE
⇒ ~ HARM. OSCIL.

Fig. 3.19 (a) Atomic displacements in long-wavelength limit. (b) Atomic displacements at wavelength $\lambda = 2a$, which corresponds to $q = \pi/a$.

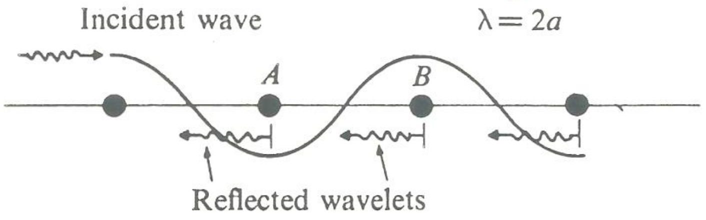


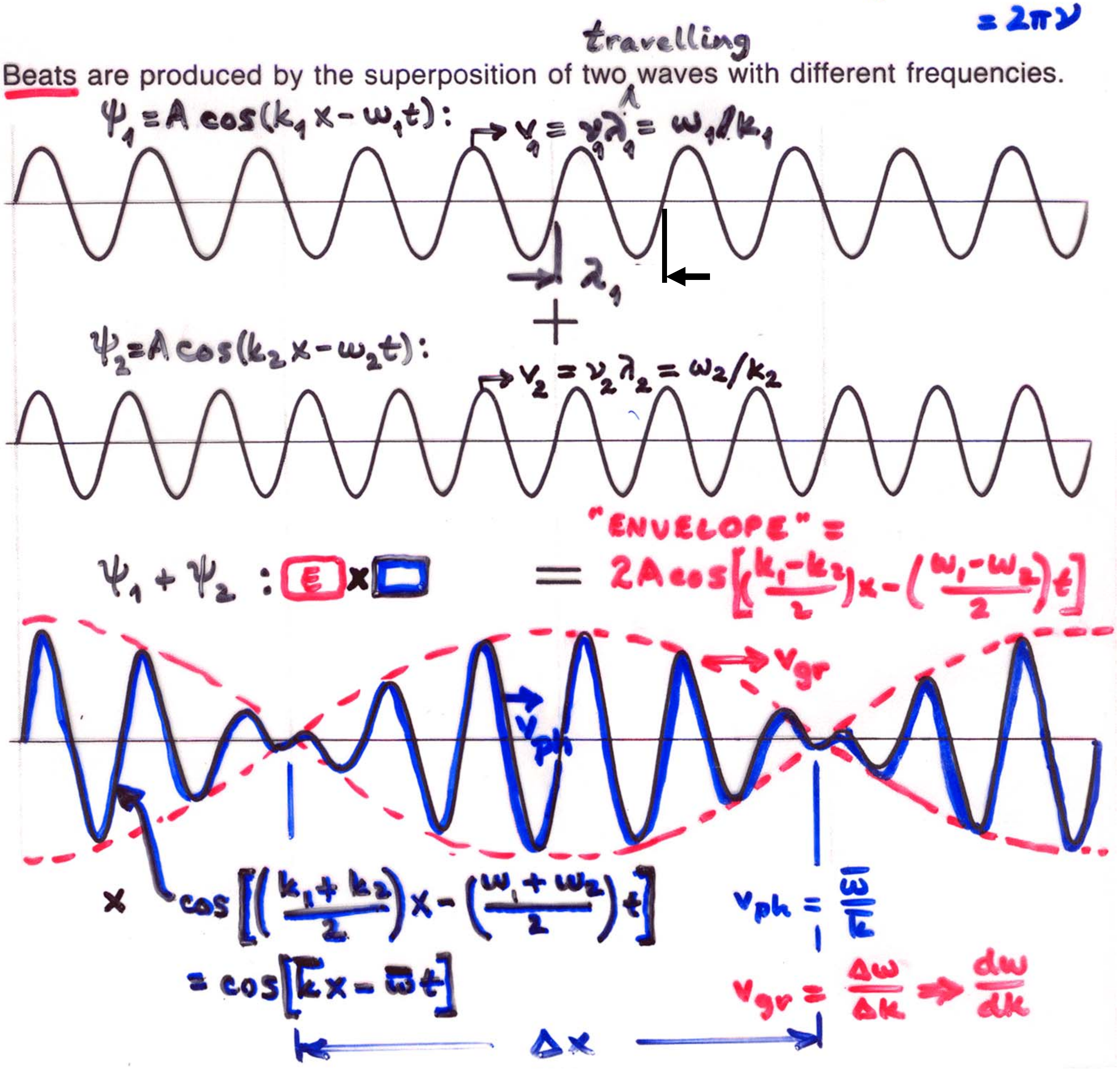
Fig. 3.20 Bragg reflection of lattice waves. ⇒

standing wave:

$$v_g = \frac{d\omega}{dq} = 0$$

Superposition of traveling waves:

$k = \frac{2\pi}{\lambda}$; $\omega = \frac{2\pi}{T} = 2\pi\nu$

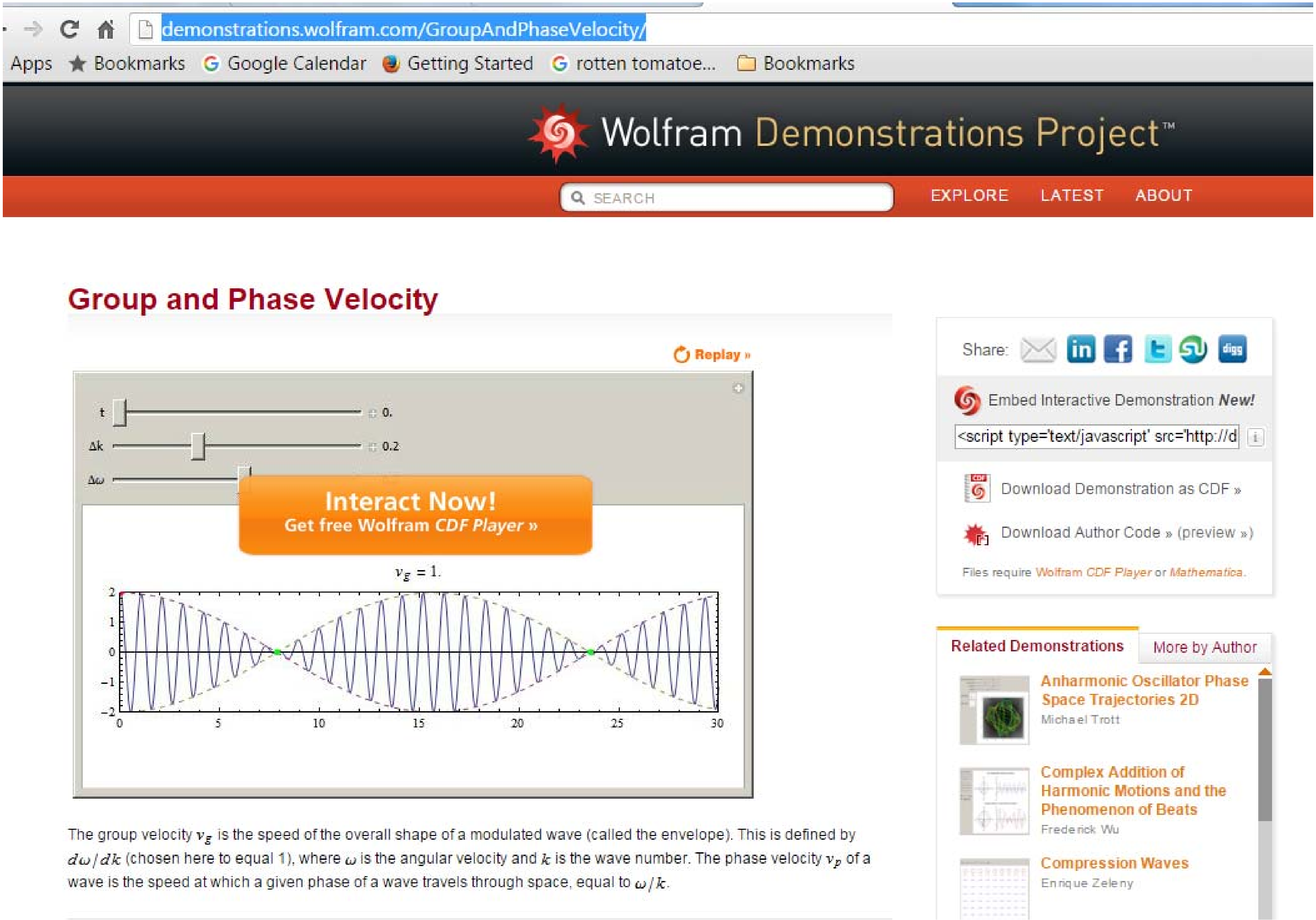


Trig. identity **:**

$$\cos a + \cos b = 2\cos\frac{1}{2}(a-b) \times \cos\frac{1}{2}(a+b)$$

E.g.--Musical notes close together in frequency

Movies at:
http://demonstrations.wolfram.com/GroupAndPhaseVelocity/



Group and Phase Velocity

The group velocity v_g is the speed of the overall shape of a modulated wave (called the envelope). This is defined by $d\omega/dk$ (chosen here to equal 1), where ω is the angular velocity and k is the wave number. The phase velocity v_p of a wave is the speed at which a given phase of a wave travels through space, equal to ω/k.

Energies of 1D vibrational waves as a function of wavevector q

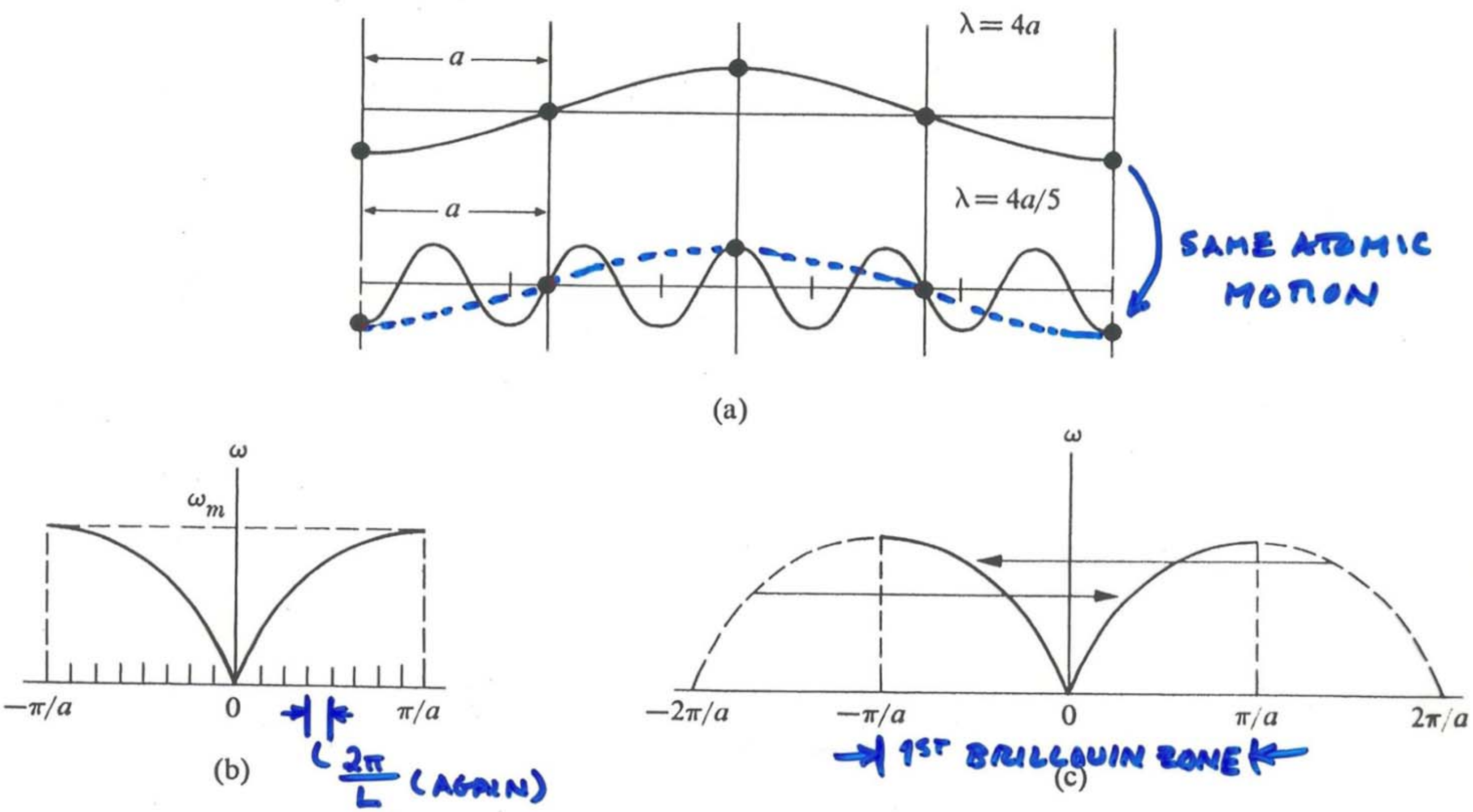


Fig. 3.21 (a) Transverse waves corresponding to $q = \pi/2a$ and $q' = q + 2\pi/a$, or $\lambda = 4a$ and $\lambda' = 4a/5$, respectively. (b) The range $-\pi/a < q < \pi/a$ is sufficient to give a unique wavelength for all physical oscillations in a one-dimensional lattice. (c) The regions in q-space connected by arrows are physically equivalent.

Energies of 1D diatomic vibrational waves: 1D chain with 2-atom basis

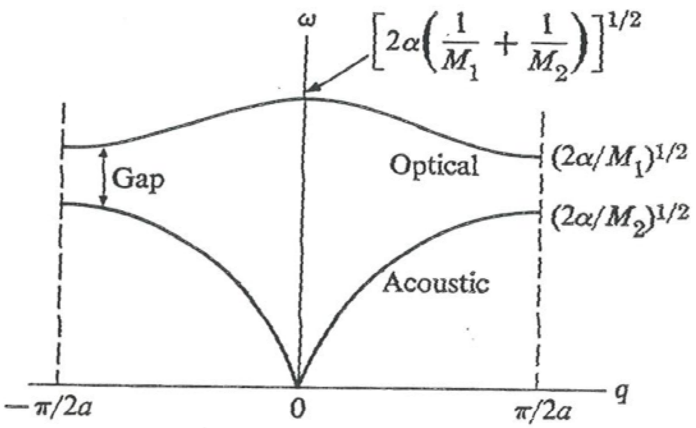


Fig. 3.23 The two dispersion branches of a diatomic lattice ($M_1 < M_2$), showing frequency gap.

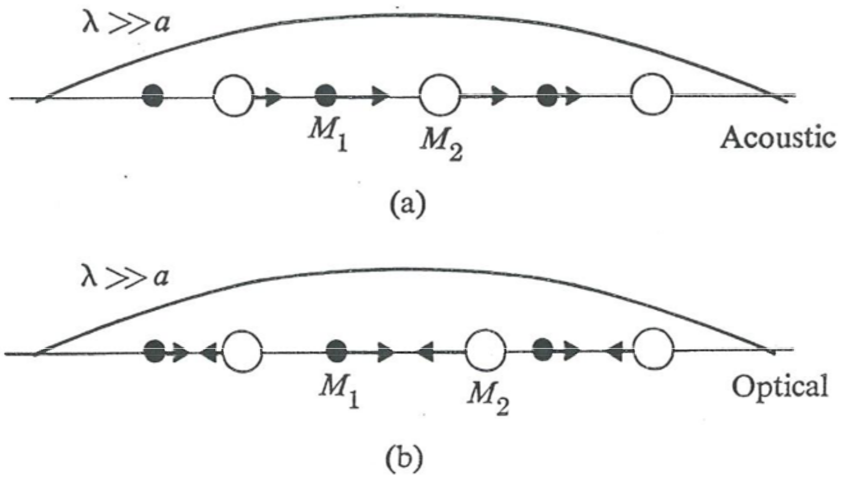
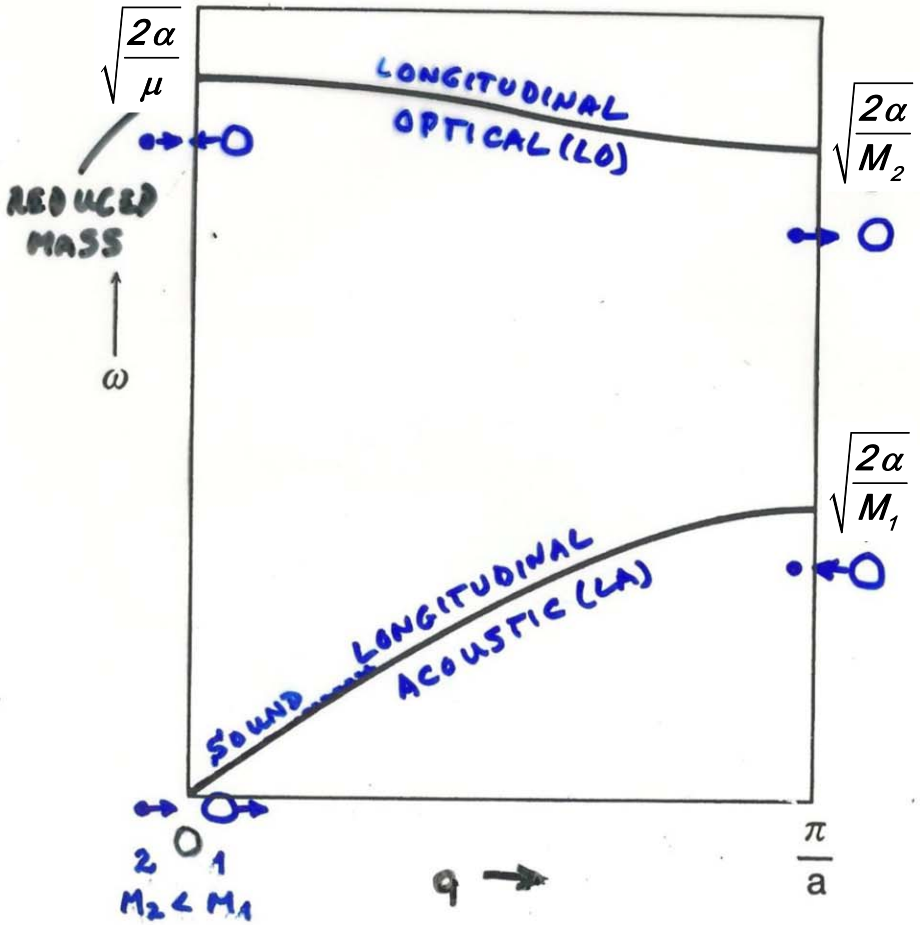


Fig. 3.24 (a) Atomic displacements in the acoustic mode at infinite wavelength ($q = 0$). (b) Atomic displacements in the optical mode at infinite wavelength.

Energies of 1D diatomic vibrational waves: optical present

4.3 The Diatomic Linear Chain 71



Light atom moves

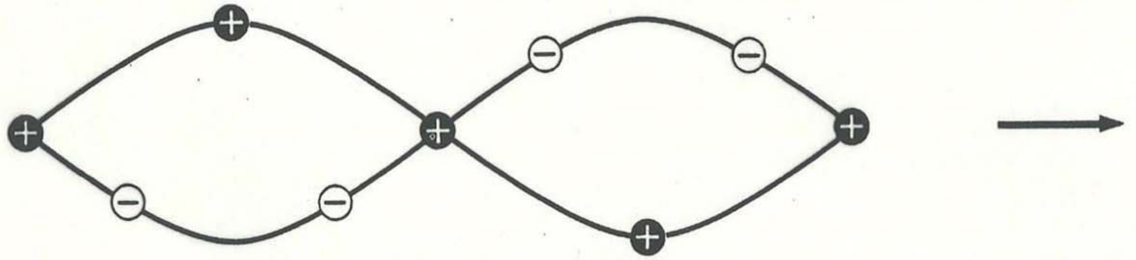
$M_1/M_2 = 5$

Heavy atom moves

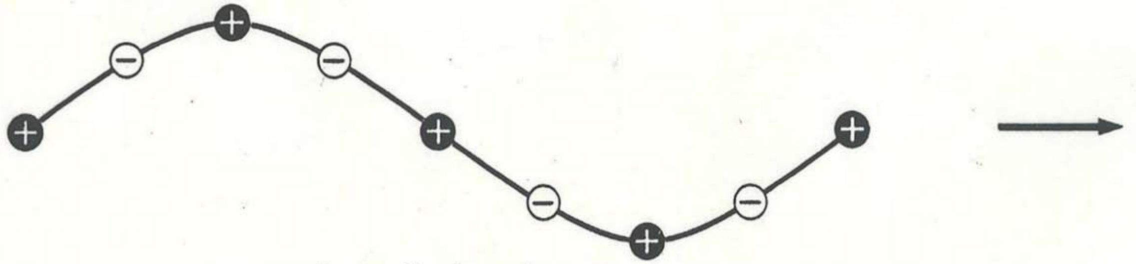
Fig. 4.3. Dispersion curve of a diatomic linear chain with a mass ratio $M_1/M_2 = 5$. With increasing mass ratio the optical branch becomes progressively flatter.

See additional discussion by Ibach and Luth, pp. 86-91

Adding more dimensions:
Transverse optical and acoustic vibrations
2D diatomic chain

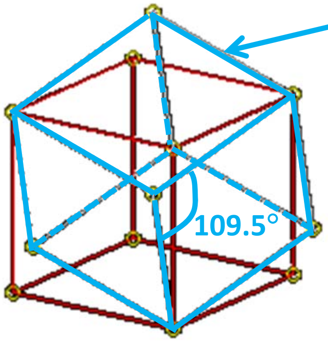


Optical mode



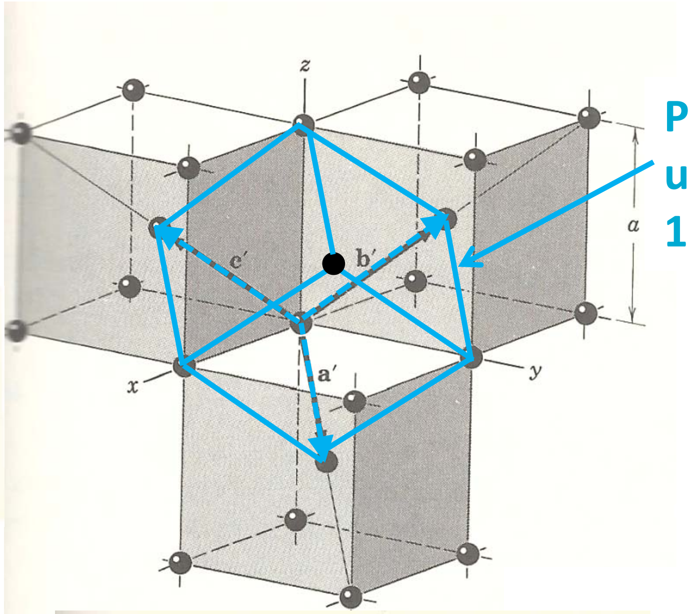
Acoustical mode

1^{st} Brillouin zone for the bcc lattice



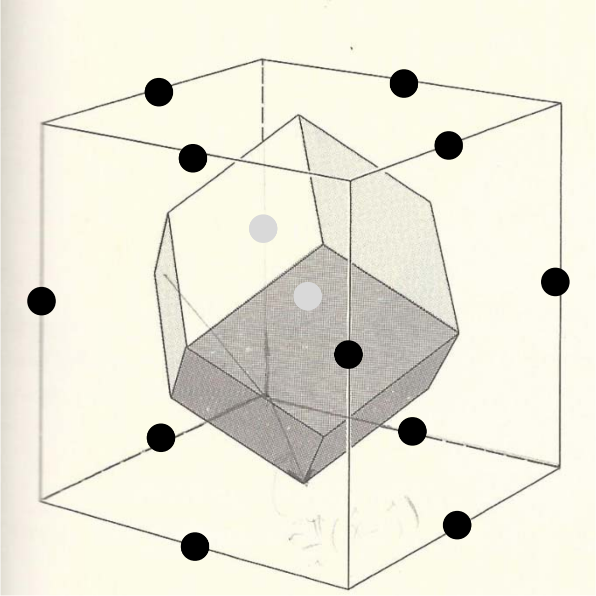
Primitive:

$$\mathbf{a}' = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})$$
$$\mathbf{b}' = \tfrac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$$
$$\mathbf{c}' = \tfrac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}})$$



Primitive unit cell: 1 atom

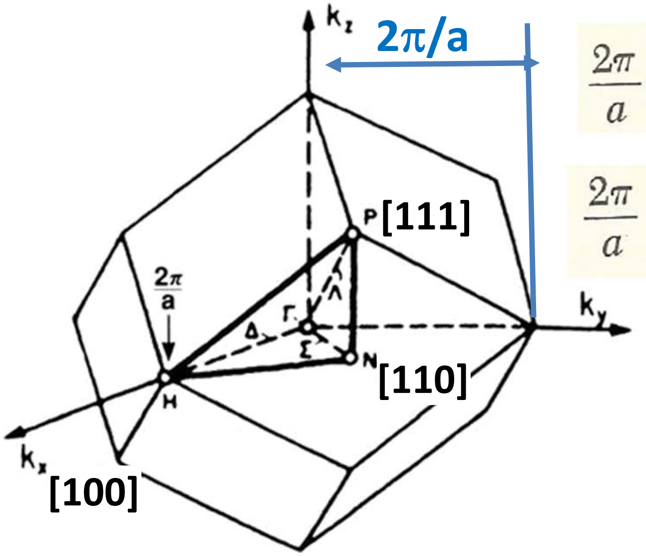
Real bcc



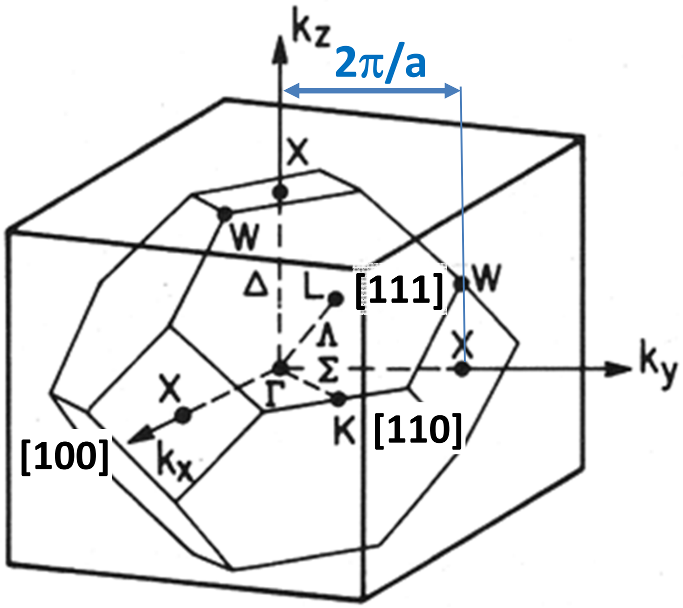
Reciprocal of bcc = fcc

Primitive: Smallest 12

$$\frac{2\pi}{a}(\pm\hat{\mathbf{x}} \pm \hat{\mathbf{y}})$$
$$\frac{2\pi}{a}(\pm\hat{\mathbf{y}} \pm \hat{\mathbf{z}})$$
$$\frac{2\pi}{a}(\pm\hat{\mathbf{x}} \pm \hat{\mathbf{z}})$$



1st Brillouin zone for the fcc lattice

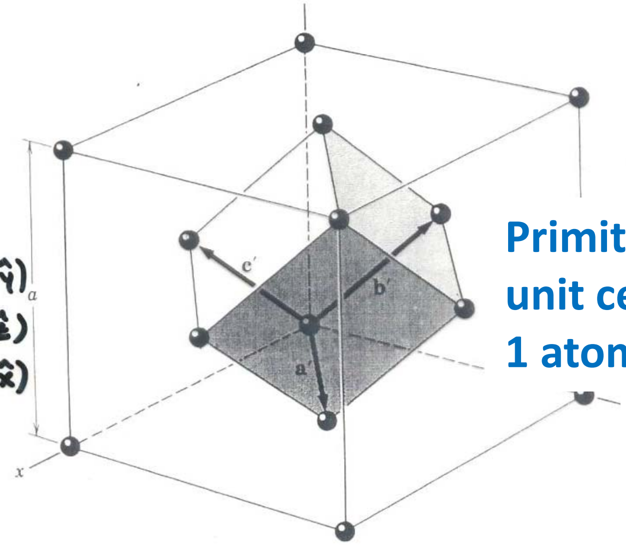


PRIMITIVE

$\bar{a}' = \frac{1}{2}a(\hat{x}+\hat{y})$

$\bar{b}' = \frac{1}{2}a(\hat{y}+\hat{z})$

$\bar{c}' = \frac{1}{2}a(\hat{z}+\hat{x})$



Real fcc

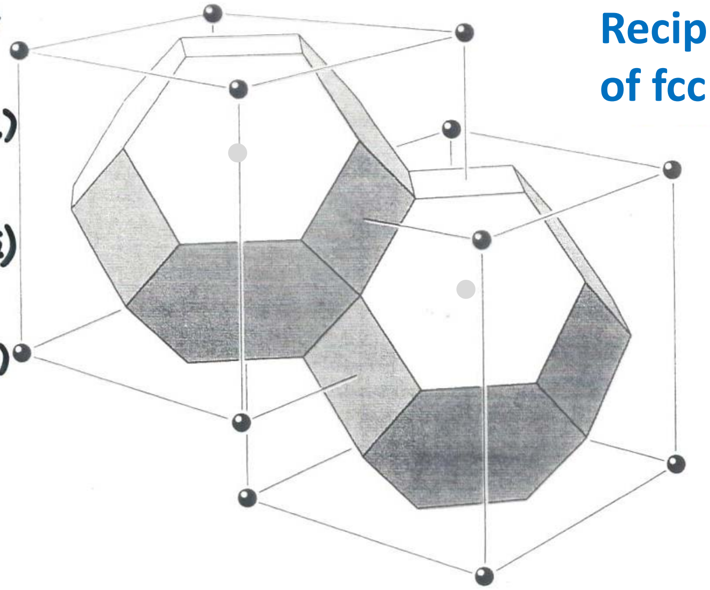
Primitive unit cell: 1 atom

PRIMITIVE

$\bar{a}^* = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

$\bar{b}^* = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$

$\bar{c}^* = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$



Reciprocal of fcc = bcc

Figure 28 Brillouin zones of the face-centered cubic lattice. The cells are in reciprocal space, and the reciprocal lattice is body-centered, as drawn.

Summing→Integrating over phonon modes

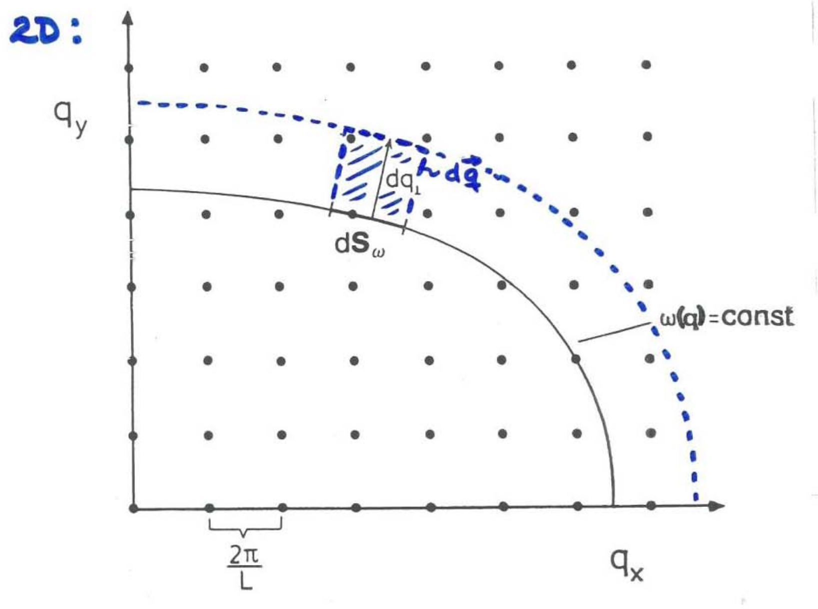


Fig. 5.1. Allowed values of *q* in reciprocal space for a square lattice. *L* is the repeat distance in real space

$$d\vec{q} = dS_\omega \, dq_\perp$$

$$d\omega = |\mathrm{grad}_q \, \omega| \, dq_\perp = |\vec{\nabla}_q \, \omega(\vec{q})| \, dq_\perp$$

NUMBER OF STATES BETWEEN ω + ω + dω =

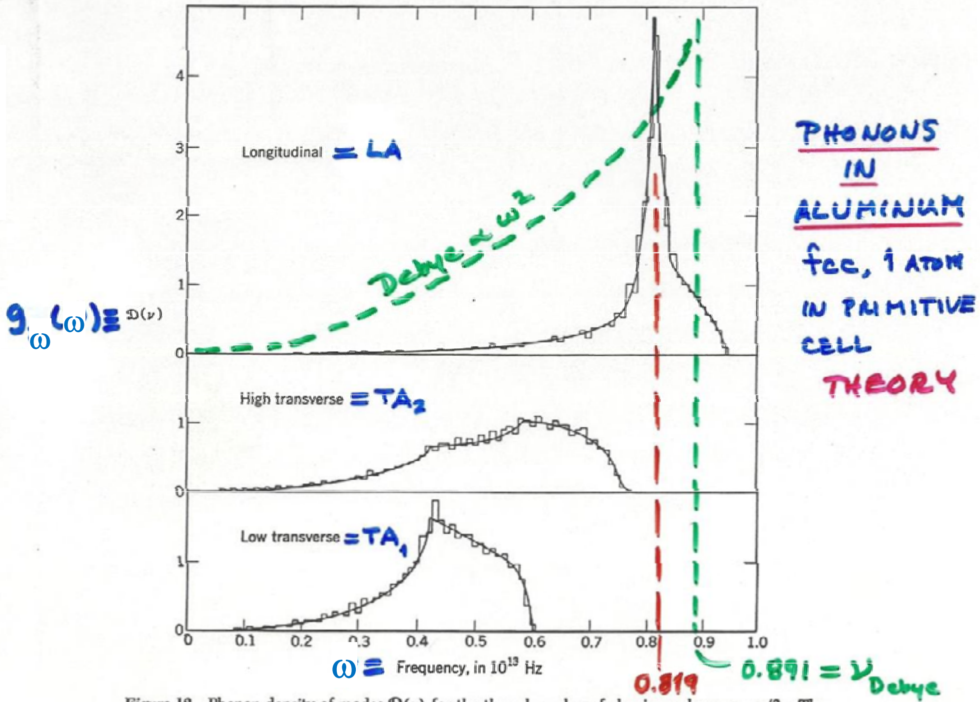
3D: $$g_\omega(\omega) \, d\omega = \frac{V}{(2\pi)^3} d\omega \int_{\omega=\mathrm{CONST}} \frac{dS_\omega}{|\mathrm{grad}_q \, \omega|}$$

+ SUM OVER BRANCHES :

LA, TA, LO, TO

From Ibach and Luth, Chapter 5

Real 3D phonon densities of states

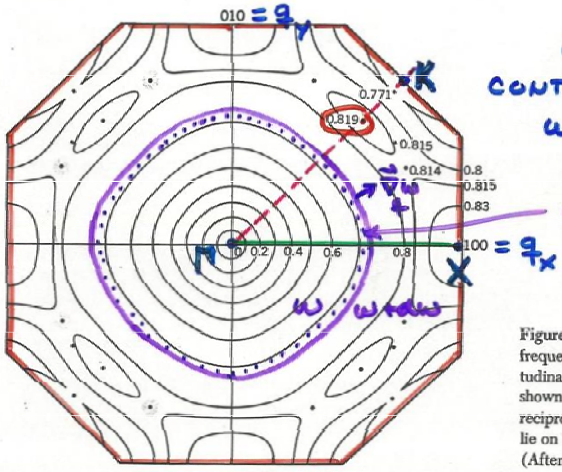


PHONONS IN ALUMINUM

fcc, 1 ATOM IN PRIMITIVE CELL

THEORY

Figure 12 Phonon density of modes $\mathfrak{D}(\nu)$ for the three branches of aluminum; here $\nu = \omega/2\pi$. The histograms are obtained from computed frequencies for 2791 wavevectors. [After C. B. Walker, Phys. Rev. 103, 547 (1956). For further results on aluminum see R. Stedman, L. Almqvist, and G. Nilsson, Phys. Rev. 162, 549 (1967).]



LA

CONTOURS OF $\omega(\vec{q})$

$$dg_\omega(\omega) \propto \frac{L^3}{(2\pi)^3} \frac{1}{|\vec{\nabla}_q \omega|} d^3q$$

Figure 13 Surfaces of constant frequency in aluminum, for longitudinal phonons. The section shown is the (100) plane of the reciprocal lattice. The gray circles lie on one set of saddle points. (After C. B. Walker.)

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Vibrational energies for real 3D crystals:

Al: fcc- no optical!

Diamond: fcc + basis- optical present

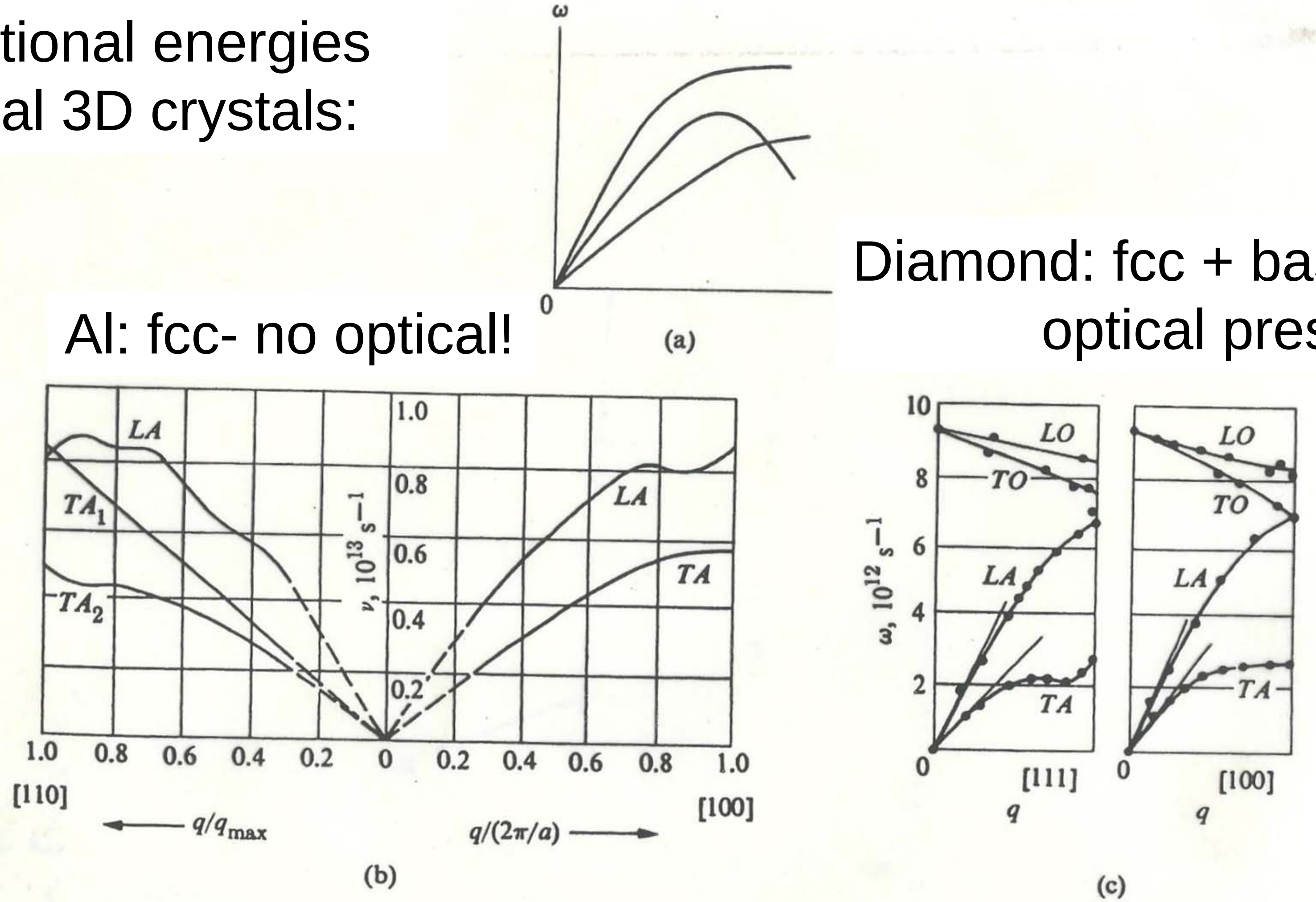
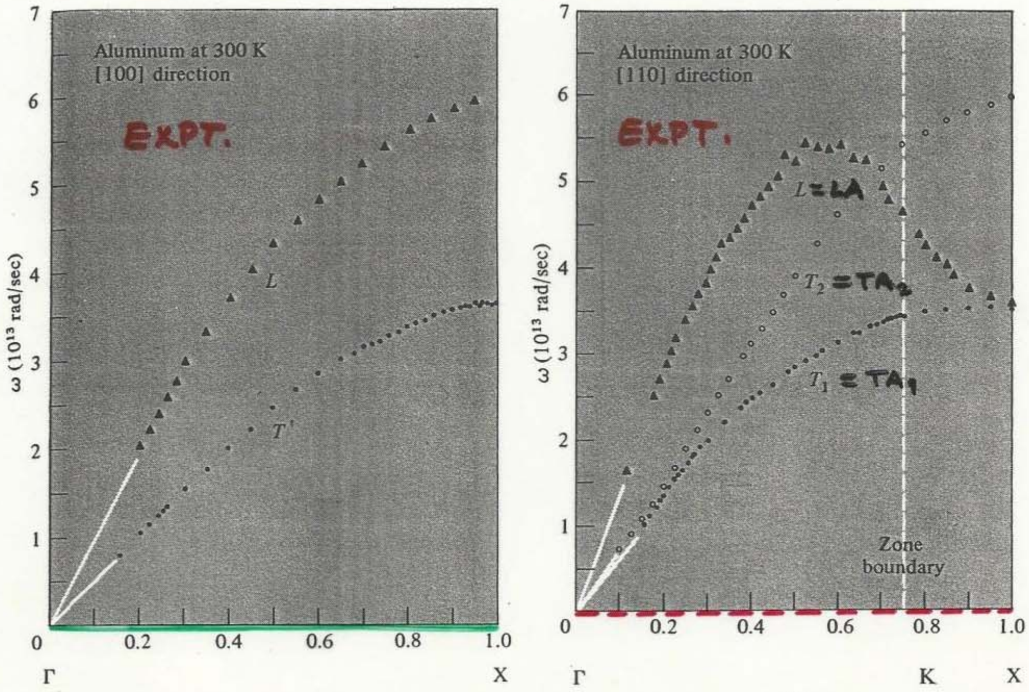


Fig. 3.25 (a) The three acoustic branches in a three-dimensional Bravais lattice. (b) Dispersion curves for Al in [100] direction (right portion) and in [110] direction, left portion. The TA branch in the [100] direction actually represents two coincident, or degenerate, branches. (Note that because each branch is individually symmetric relative to the origin, only half of each branch is plotted.) (c) Dispersion curves of Ge in the [100] and [111] directions.

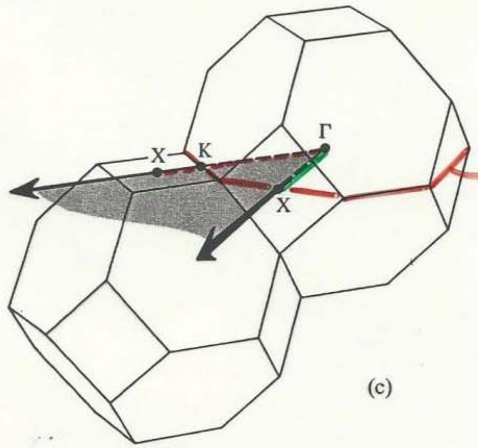
Phonons in aluminum-fcc, no optical

Neutron Scattering by a Crystal 475



(a)

(b)



(c)

COMPARE TO
CALCULATED
CROSS SECTION
IN THIS PLANE

Vibrational energies for bcc tungsten-no optical

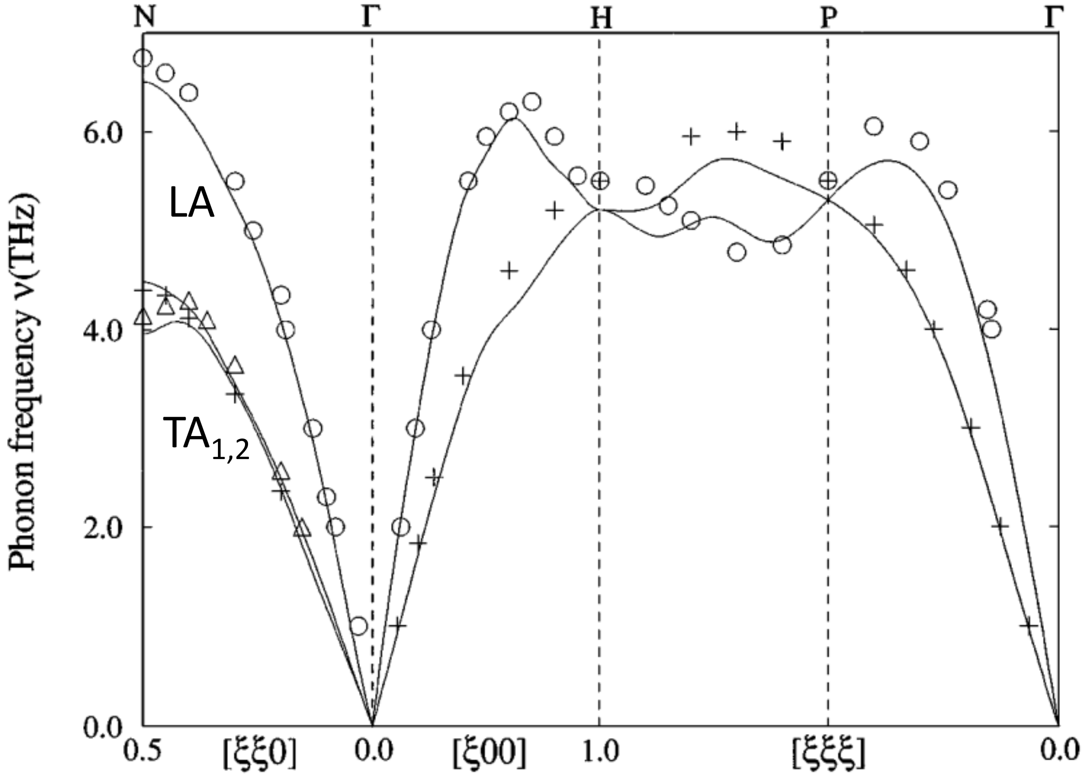
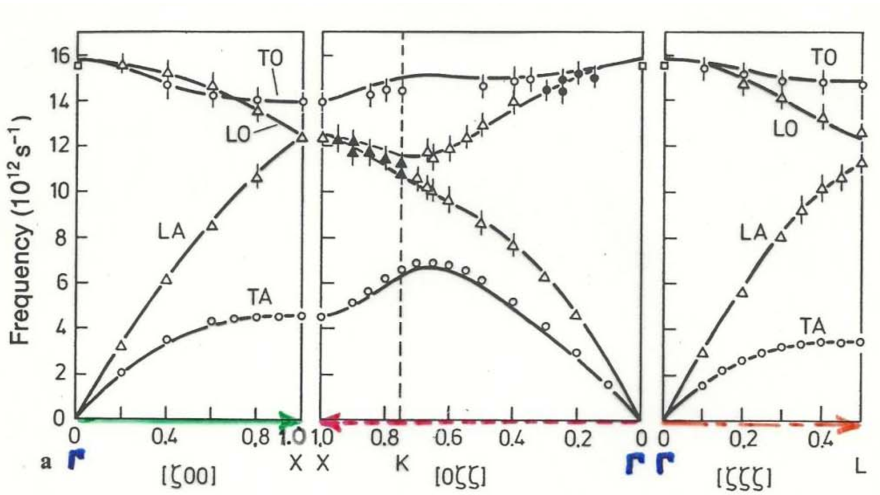
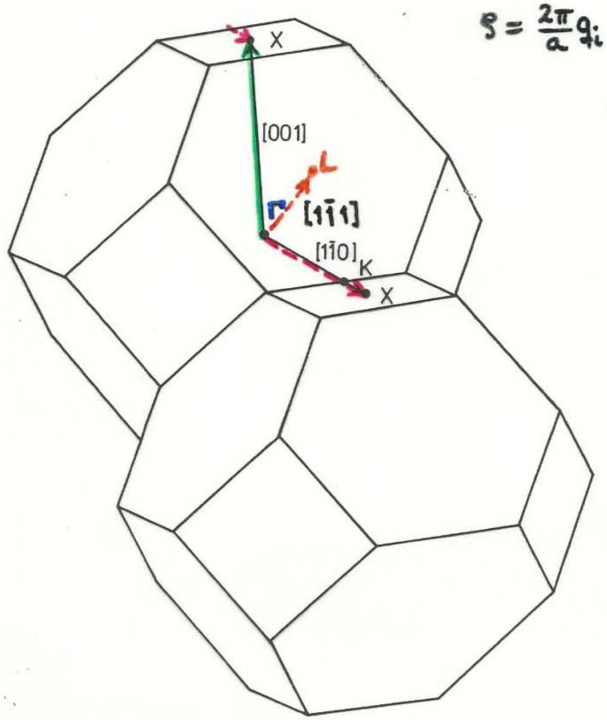


FIG. 1. Experimental [18] (symbols) and calculated (solid lines) phonon frequencies of bcc W at the equilibrium volume.

Phonons in a diamond lattice: Si- fcc + 2-atom basis, optical present



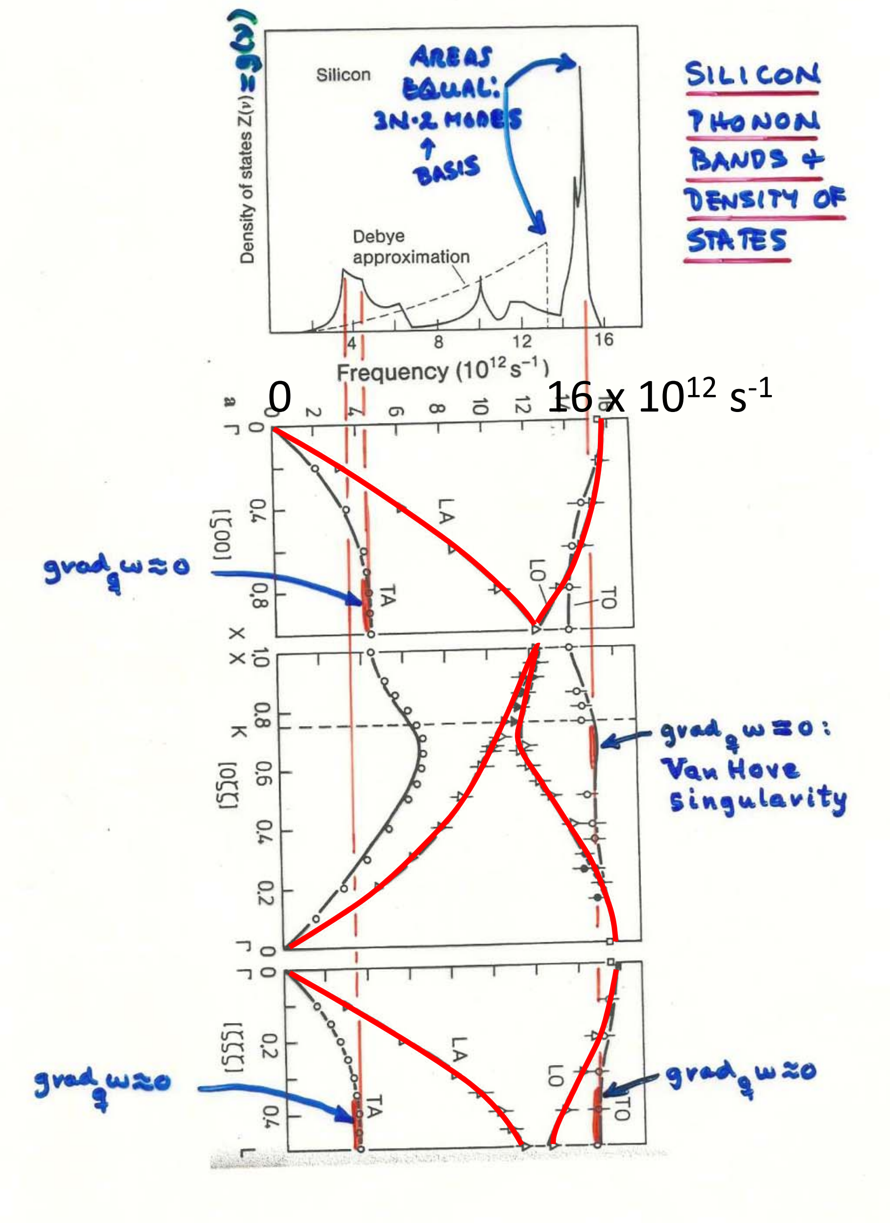
$ς = \frac{2\pi}{a} q_i$



VIBRATIONS IN A
REAL 3D CRYSTAL:
Si = DIAMOND =
fcc + 2-atom
basis

Phonons in silicon

Conversion
: 1.24 meV
= 300 GHz
= 3×10^{11} s^{-1}



$(2)g =$

AREAS EQUAL: 3N·2 MODES
↑
BASIS

SILICON PHONON BANDS + DENSITY OF STATES

0 16×10^{12} s^{-1}

$\text{grad}_q\,\omega \approx 0$

$\text{grad}_q\,\omega \approx 0$: Van Hove singularity

$\text{grad}_q\,\omega \approx 0$

$\text{grad}_q\,\omega \approx 0$

Phonons in diamond

0 387×10^{11}

$= 38.7\times10^{12}$ s^{-1} (higher!)

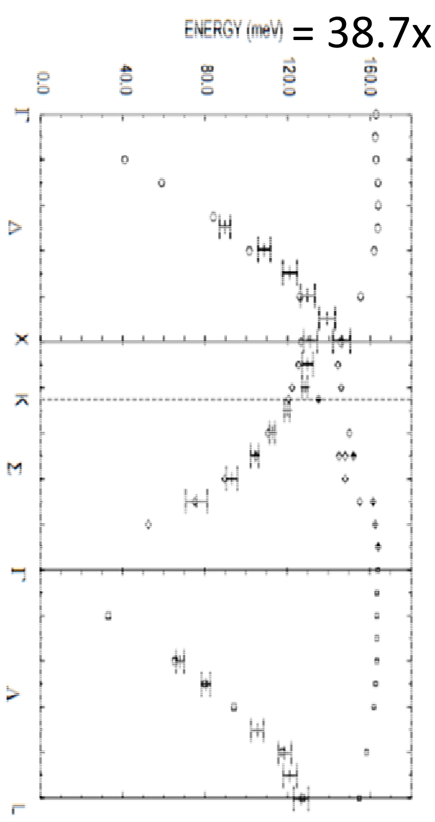
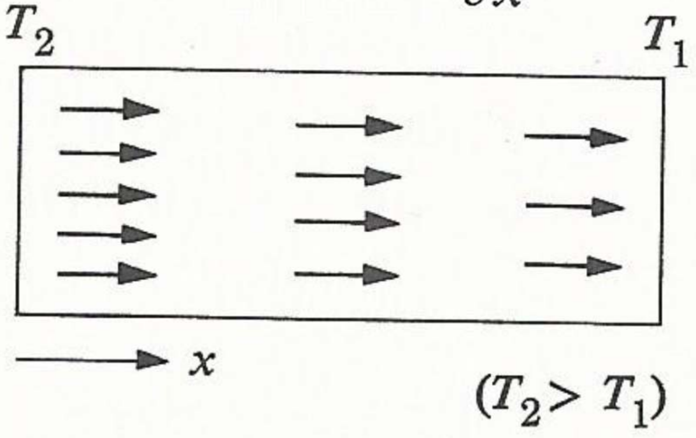


FIG. 2. Longitudinal phonon branches along Δ, Σ, and Λ: Symbols without error bars are HRIXS data; symbols with error bars were obtained by inelastic neutron scattering [14,15].

Thermal conductivity by phonons and Fick's Law

$$Q = -K\frac{\partial T}{\partial x}$$



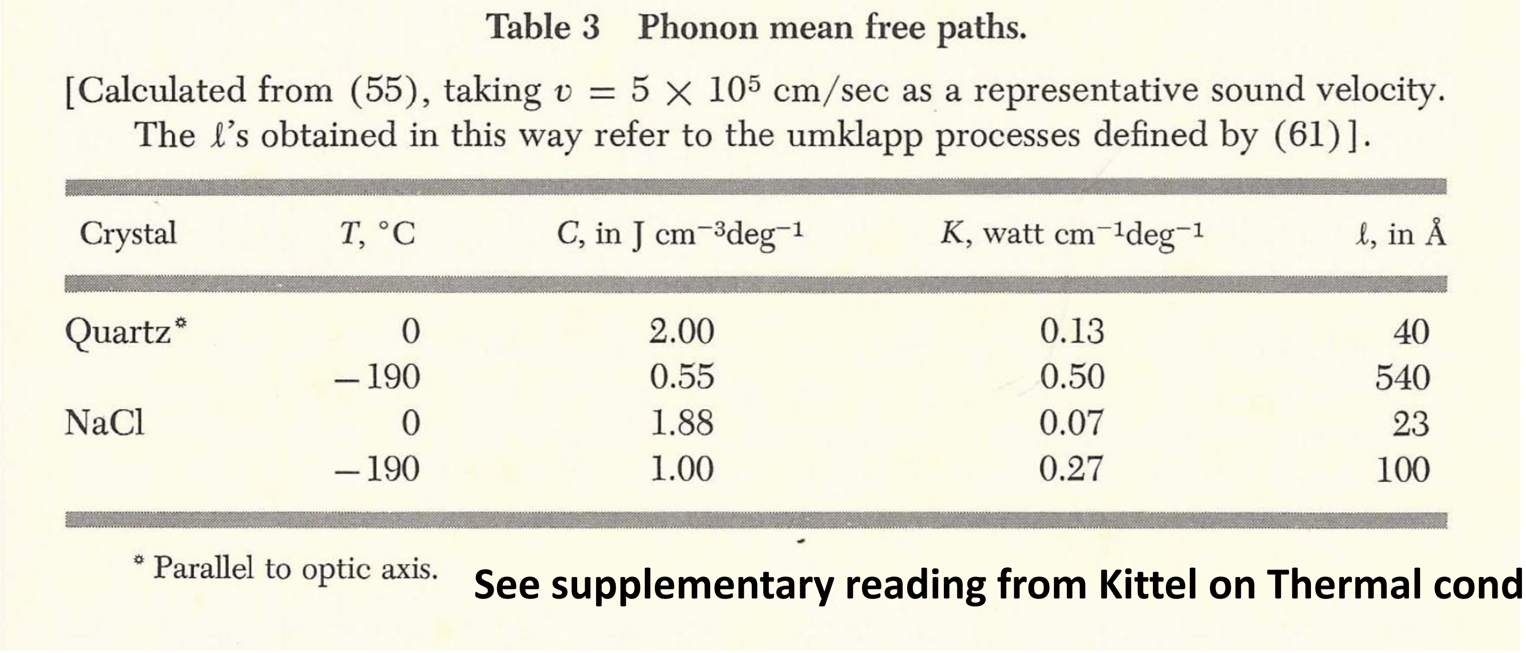


Table 3 Phonon mean free paths.

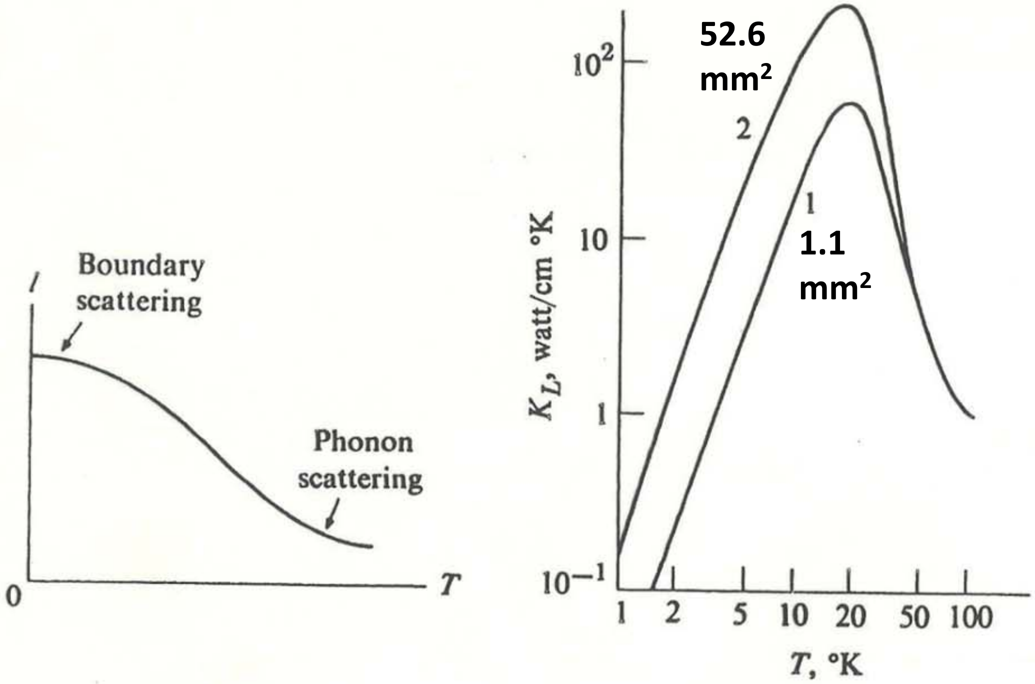
[Calculated from (55), taking $v = 5 \times 10^5$ cm/sec as a representative sound velocity. The ℓ's obtained in this way refer to the umklapp processes defined by (61)].

Crystal	T, °C	C, in J cm^{-3}deg^{-1}	K, watt cm^{-1}deg^{-1}	ℓ, in Å
Quartz*	0	2.00	0.13	40
	−190	0.55	0.50	540
NaCl	0	1.88	0.07	23
	−190	1.00	0.27	100

* Parallel to optic axis.

See supplementary reading from Kittel on Thermal conductivity

Thermal conductivity by phonons and Fick’s Law: Phonon and boundary scattering



(a) (b)

Fig. 3.32 Thermal conductivity of isotopically pure crystals of LiF. Curve 1 is for a bar of cross section 1.23 × 0.91 mm. Curve 2 is for a bar of cross section 7.55 × 6.97 mm. (After P. D. Thatcher, Phys Rev. **156**, 975 (1967).)

Phonon scattering processes: normal and umklapp

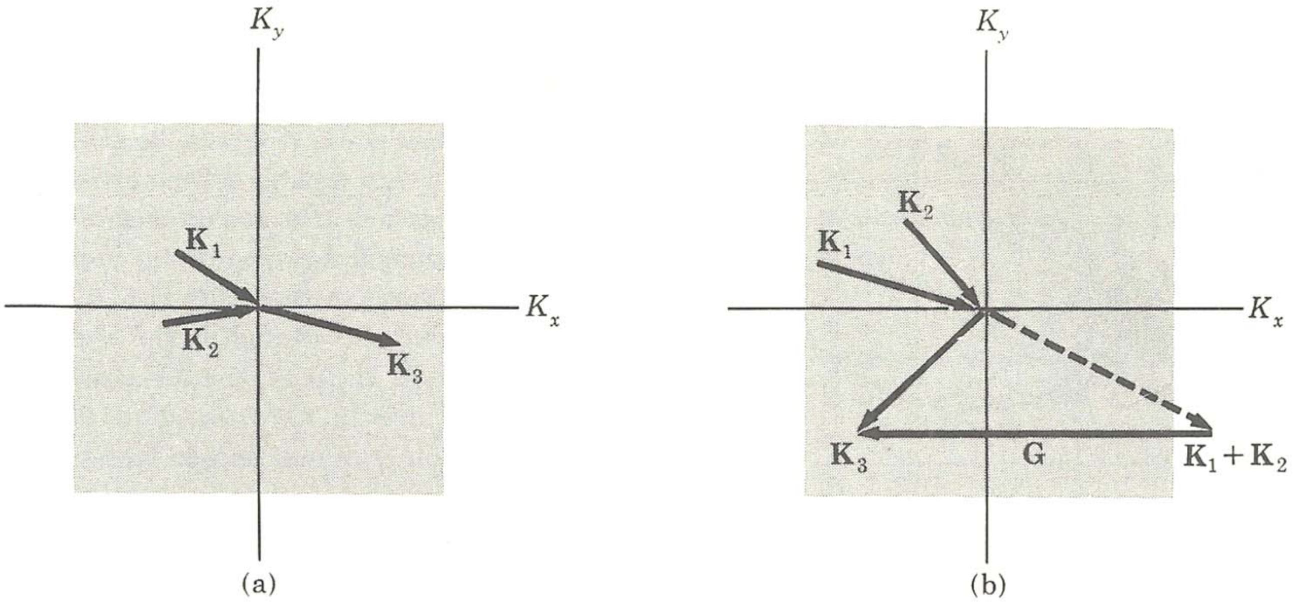
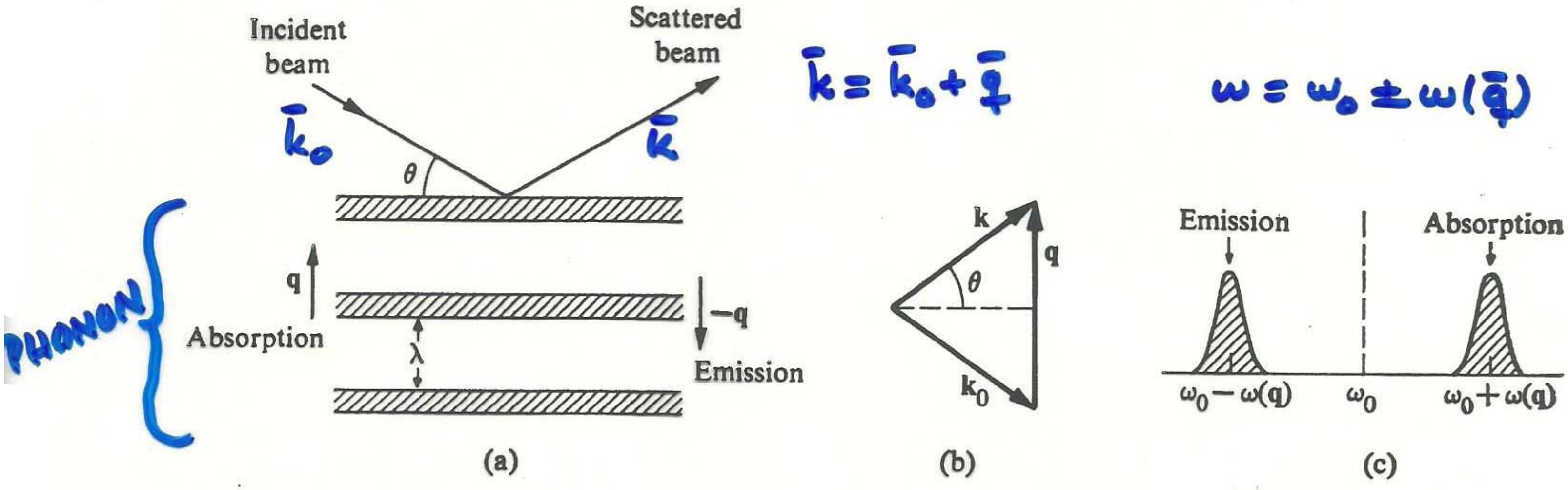


Figure 22 (a) Normal $\mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3$ and (b) umklapp $\mathbf{K}_1 + \mathbf{K}_2 = \mathbf{K}_3 + \mathbf{G}$ phonon collision processes in a two-dimensional square lattice. The square in each figure represents the first Brillouin zone in the phonon $\mathbf{K}$ space; this zone contains all the possible independent values of the phonon wavevector. Vectors $\mathbf{K}$ which have arrowheads at the center of the zone represent phonons absorbed in the collision process; those with arrowheads away from the center of the zone represent phonons emitted in the collision. We see in (b) that in the umklapp process the direction of the x-component of the phonon flux has been reversed. The reciprocal lattice vector $\mathbf{G}$ as shown is of length $2\pi/a$, where a is the lattice constant of the crystal lattice, and is parallel to the $\mathbf{K}_x$ axis. For all processes, N or U, energy must be conserved, so that $\omega_1 + \omega_2 = \omega_3$.

Inelastic x-ray scattering by phonons: like a doppler shift in scattering



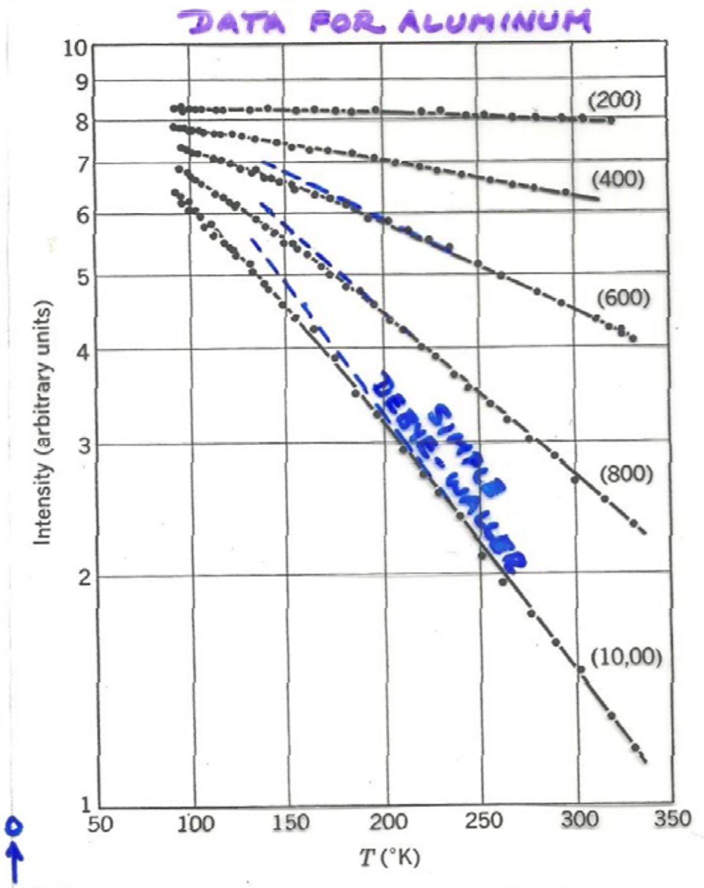
$\bar{k} = \bar{k}_0 + \bar{q}$

$\omega = \omega_0 \pm \omega(\bar{q})$

Fig. 3.34 Scattering of x-rays by phonons. (a) The vibrating lattice acts as a set of planes at spacing equal to λ. Absorption of a phonon **q** and emission of a phonon $-\mathbf{q}$ lead to the same momentum conservation, and hence the two processes are observed simultaneously at the detector. Their frequencies are different, however. (b) Conservation of momentum for x-ray photon–phonon collision. (c) Shifted x-ray frequencies.

Recall: Vibrational effects on diffraction: the Debye-Waller factor

Vibrations smear positions, decrease diffraction→phonons



See supplementary reading from Kittel on Debye-Waller factor

0 ↑ RESIDUAL ZERO-POINT VIBRATION

$$I_{hk\ell}(T) = I_{hk\ell}(\text{rigid lattice})\exp[-\frac{1}{3} < u^2 > G^2_{hk\ell}],$$

if harmonic oscillator with mass M and frequency $\omega = \sqrt{\frac{k}{M}}$,

$$= I_{hk\ell}(\text{rigid lattice})\exp[\frac{-k_B T G^2_{hk\ell}}{M\omega^2}]$$