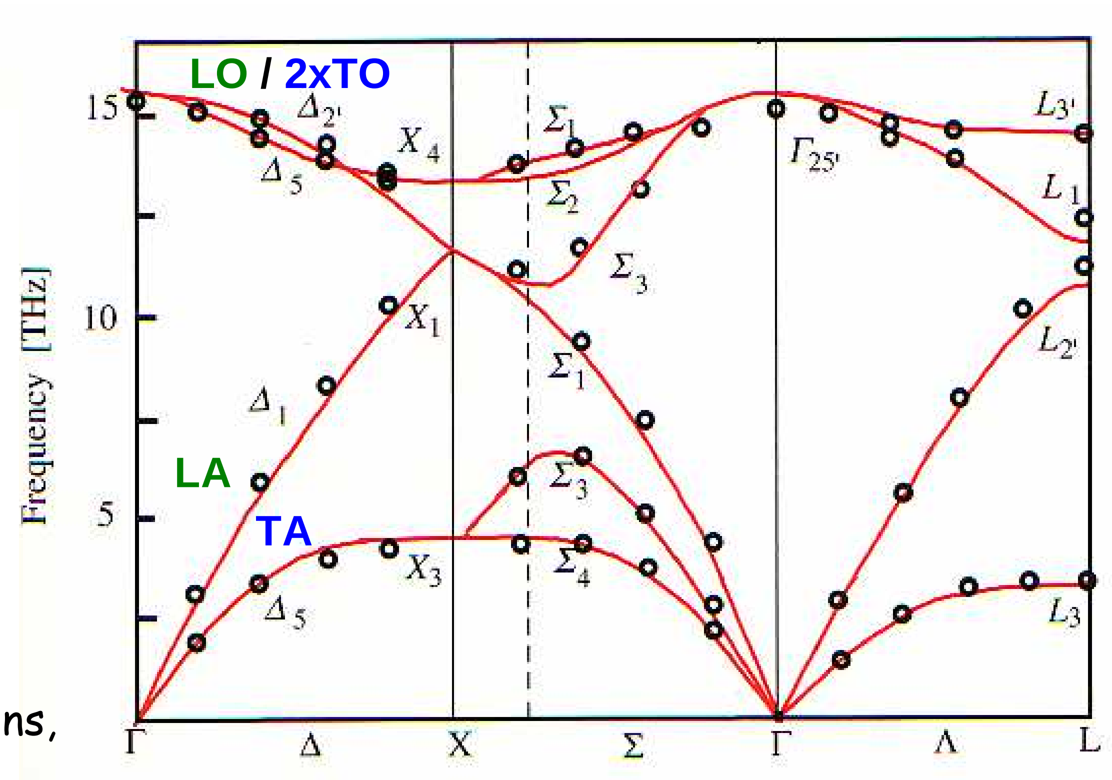
Phonon dispersion relations for Silicon

Note:

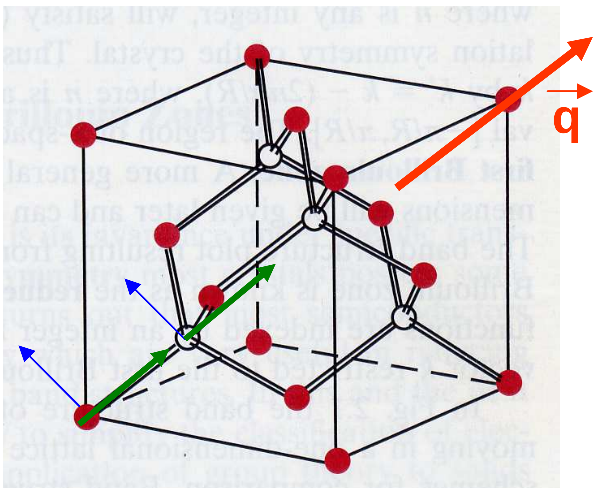
- LA (compression wave) alsways higher frequency than TA (shear wave)
- LO + 2 x TO degenerate at Γ^+
- 2xTO stay degenerate along the symmetry lines Δ and Λ.



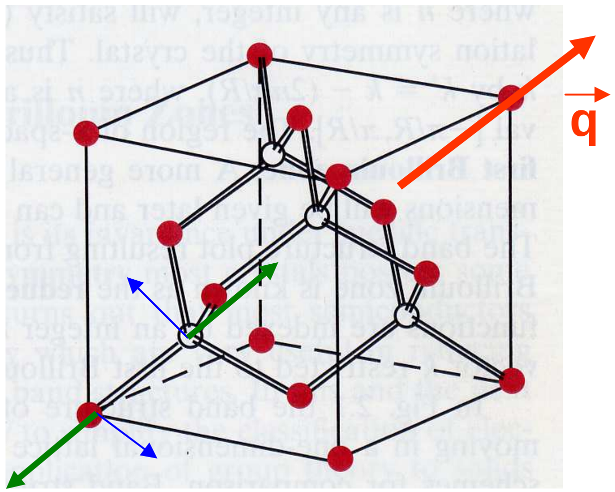
For q along high-symmetry directions, modes can be classified as

Lognitudinal L
or
Transverse T

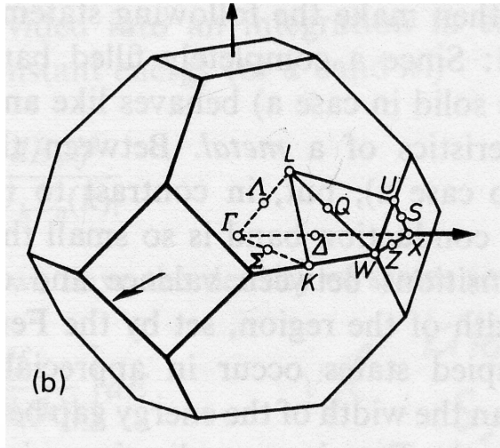
Accoustic modes



Optical modes

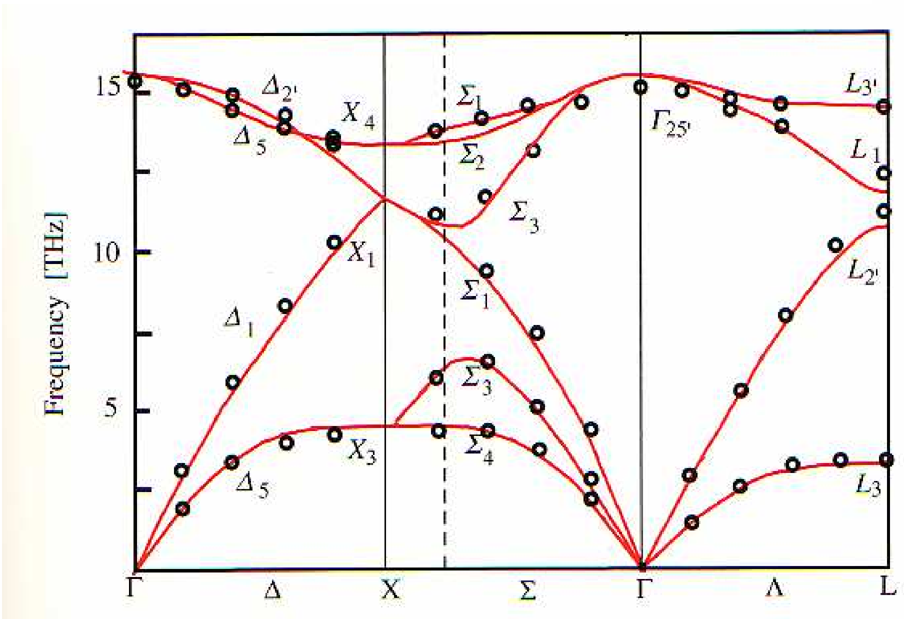


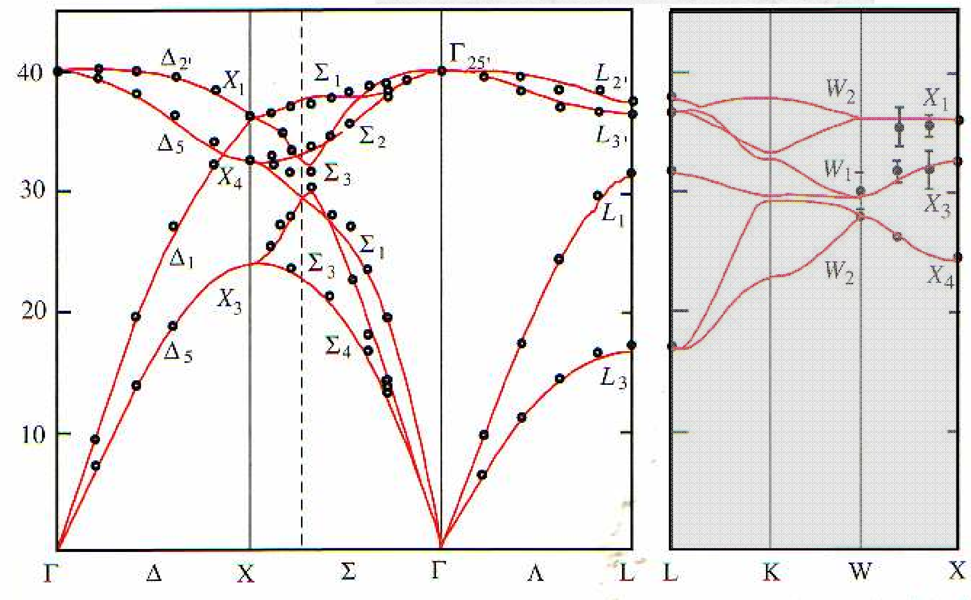
Comparison: Silicon and Diamond



Si

Diamond



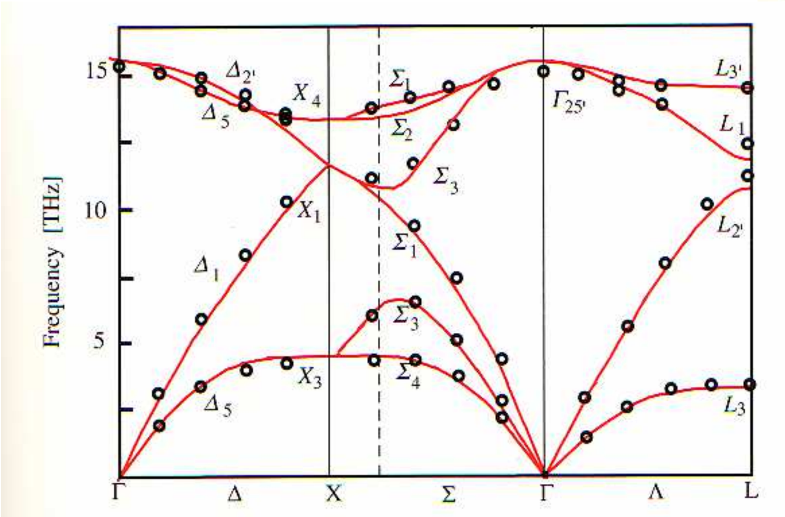


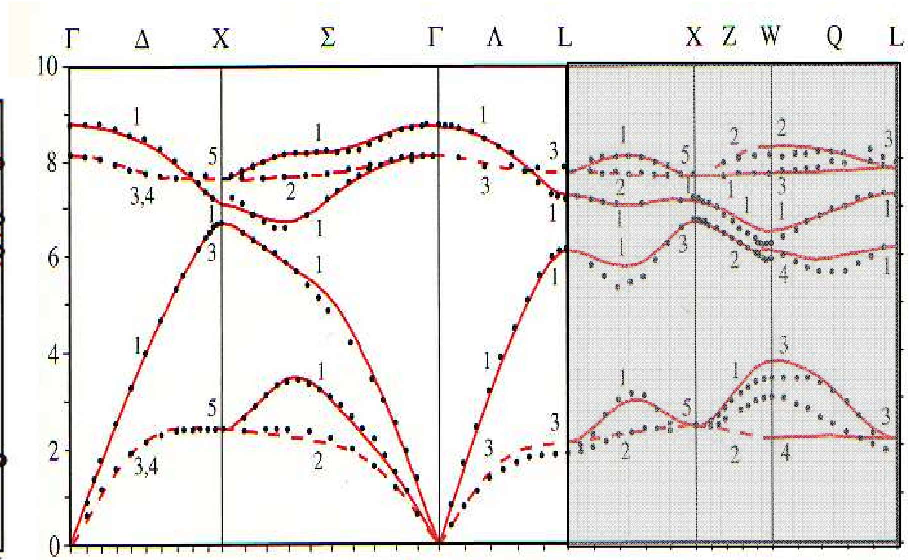
M_{Si} = 28 u = $1{,}5^2$ M_C

M_C = 12 u

→ C not only lighter than Si, but in addition, C-C-bonds much stronger than Si-Si bonds!

Comparison: Silicon and GaAs





<u>Si</u>:

M_{Si}=28 u

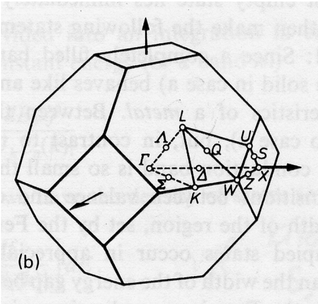
LO/TO degenerate at Γ^{+}

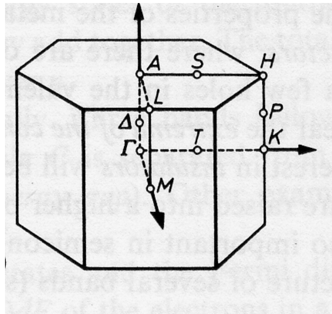
<u>GaAs</u>:

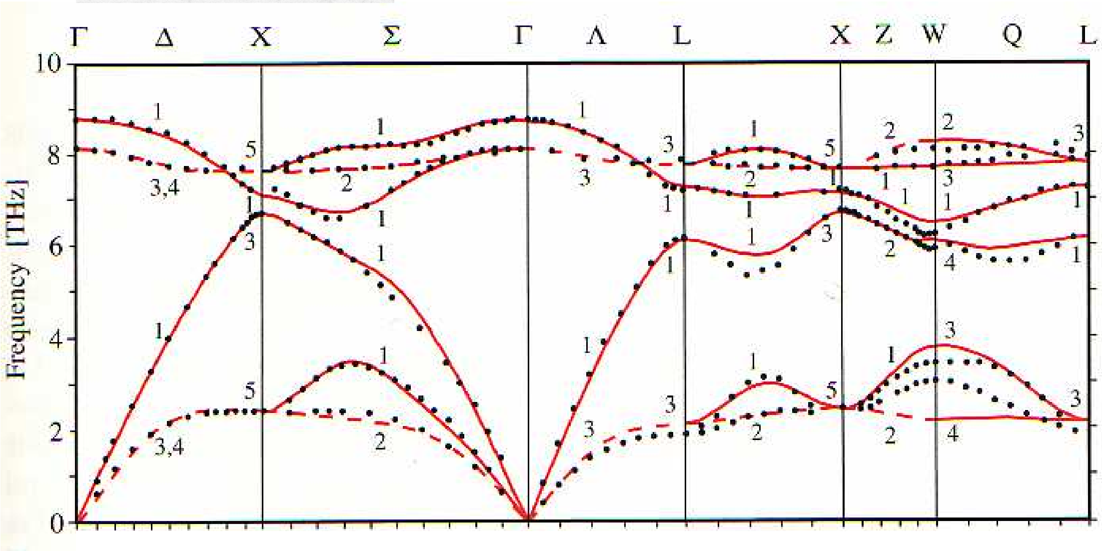
M= 68 u = $1{,}5^{2}$ M_{Si}

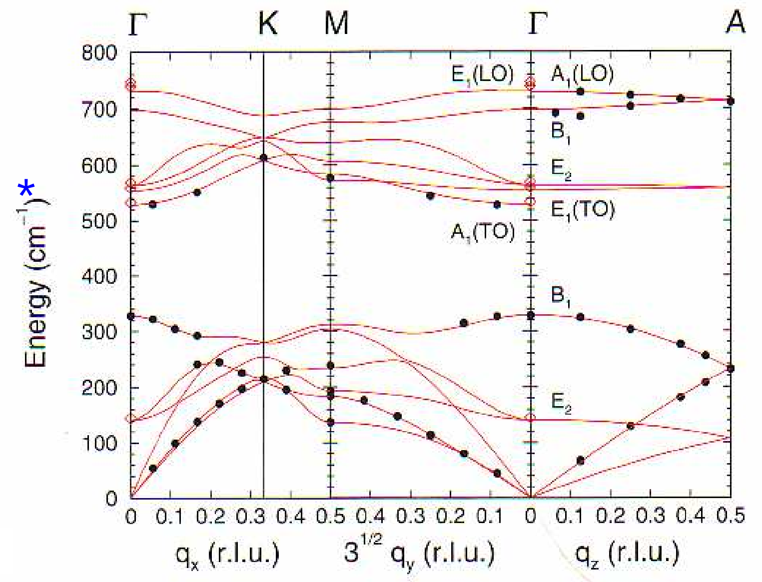
LO/TO split at Γ^{+} due to inequivalent atoms in the base!

Comparison: GaAs (Zincblende) and GaN (Wurtzith)









* common frequency unit in IR spsectroscopy:

$\frac{E}{hc} = \frac{f}{c}$; unit cm^{-1} also named ‚Kayser‘

With increasing mass ratio:

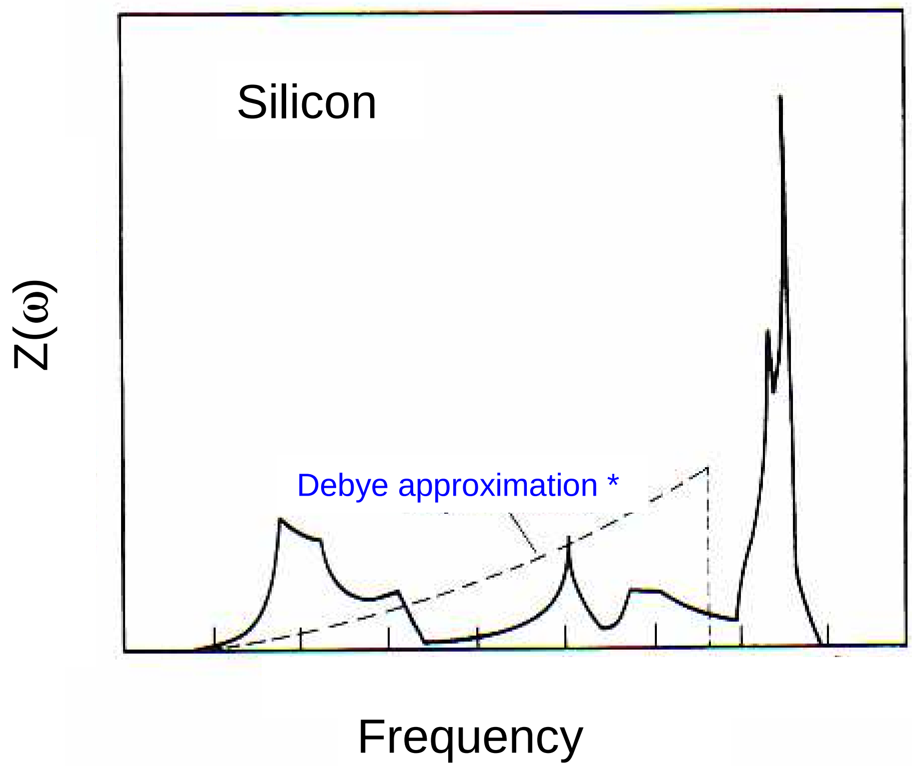
- Larger frequency (=energy) gap between optical and acoustic branches
- Otical branches get flatter!

→ Already reproduced by the ‚linear chain model‘ (see, e.g. Ibach)

Phonon Density of States

For thermodynamic phenomena related to phonons, a less specific characterization of the phonons is in many cases sufficient:
The phonon Density of States Z(ω). Definition like for electrons:

$$Z(\omega) = \frac{1}{(2\pi)^3} \sum_n \int_{\substack{\text{constant} \\ \text{frequency surface}}} \frac{dA_q}{\left|\vec{\nabla}_{\vec{q}}\,\omega_n(\vec{q})\right|}$$



*Debye approximation for the phonons :
Three phonon branches with linear dispersion relations $\omega_n(\vec{q}) = v_n \cdot |\vec{q}|$ corresponding to the low-frequency ranges of the TA and LA branches and a common cut-off frequency such that the correct total number of phonon modes (**including the optical ones**) is reproduced.

$$\longrightarrow N_n(\omega) = \frac{1}{(2\pi)^3} \cdot \frac{4}{3}\pi\left(\frac{\omega}{v_n}\right)^3 \longrightarrow Z_n(\omega) = \frac{dN_n}{d\omega} = \frac{4\pi}{(2\pi)^3 v_n^{\ 3}} \cdot \omega^2$$

and thus for n = TA, TA, TO

$$Z(\omega) = \frac{4\pi}{(2\pi)^3} \cdot \left(\frac{2}{v_{TA}^{\ 3}} + \frac{1}{v_{LA}^{\ 3}} \right) \cdot \omega^2$$