Phonons in 3D

$$\bar{R}_\ell = \bar{R}_{n,\kappa} = \bar{R}^0_n + \bar{R}^0_\kappa + \bar{u}_{n\kappa}$$

- $\bar{R}_\ell = \bar{R}_{n,\kappa}$: Instantaneous position of atom $\ell = (n,\kappa)$ (unit cell ← n; basis atom ← κ)
- $\bar{R}^0_n$: equilibrium position of unit cell
- $\bar{R}^0_\kappa$: equilibrium position of basis pt.
- $\bar{u}_{n\alpha}$: displacement of atom from equilibrium

Harmonic Approximation:

$$\mathcal{H} = \sum_{n,\alpha} \frac{\bar{P}^2_{(n,\kappa)}}{2M_\alpha} + \sum_{n,n'} \sum_{\alpha,\alpha'} \sum_{\mu,\mu'} \Phi^{0\,\mu,\mu'}_{\alpha,\alpha'}(n,n')\, u^\mu_\alpha(n)\, u^{\mu'}_{\alpha'}(n')$$

- $\sum_{n,\alpha}$: sum over unit cells, $n = 0, \cdots N$
- $\sum_{n,n'} \sum_{\alpha,\alpha'}$: sum over basis atoms, $\kappa = 1 \cdots N_b$
- $\sum_{\mu,\mu'}$: sum over dimensions, $\mu = x, y, z$

$\Phi^{0\,\mu,\mu'}_{\alpha,\alpha'}(n,n')$ → force induced on the (n,α) atom in the μ-direction, due to a unit displacement of the (n',α') atom in the μ'-direction

→ we can follow the same procedure as before

Once again, we obtain coupled differential equations. Solutions for displacement take the form:

$$u_\alpha^\mu(n,t) = u_\alpha^\mu(n)\frac{1}{\sqrt{M_\alpha}} e^{-i\omega t}$$

$$= \frac{\epsilon_\alpha^\mu}{\sqrt{M_\alpha}} e^{ik\cdot\bar{R}_n^\circ} e^{ik\cdot\bar{R}_\alpha^\circ} e^{-i\omega t}$$

$e^{ik\cdot\bar{R}_n^\circ} e^{ik\cdot\bar{R}_\alpha^\circ}$: geometric phase factor (depends on position in lattice)

$e^{-i\omega t}$: oscillatory term

- the result is a characteristic eqn defining the Dynamical Matrix:

$$\omega^2 \epsilon_\alpha^\mu = \sum_{\alpha',\mu'} D_{\alpha,\alpha'}^{\mu,\mu'} \epsilon_{\alpha'}^{\mu'} \Rightarrow \omega^2 \epsilon(k) = D(k)\,\epsilon(k)$$

Dynamical Matrix elements:

$$D_{\alpha,\alpha'}^{\mu,\mu'}(k) = \frac{1}{\sqrt{M_\alpha M_{\alpha'}}} \sum_{n'} \varphi_{\alpha,\alpha'}^{\mu,\mu'}(n,n') e^{ik\cdot(\bar{R}_n^\circ - \bar{R}_{n'}^\circ)}$$

$m = n - n'$

$$D_{\alpha,\alpha'}^{\mu,\mu'}(k) = \frac{1}{\sqrt{M_\alpha M_{\alpha'}}} \sum_m \varphi_{\alpha,\alpha'}^{\mu,\mu'}(m) e^{ik\cdot\bar{R}_m^\circ}$$

- Notice now that $\hat{D}(k)$ is a $3N_b \times 3N_b$ matrix

$\Rightarrow N_b$ = # of atoms in unit cell (in basis)

- Evidently, we will have $3N_b$ independent solutions for $\omega^2(k)$, i.e. $3N_b$ phonon branches.

- the terms ϵ_α^m represent the amplitude normalization of the vibration.

- in our general equation: $\omega^2 \epsilon(k) = \hat{D}(k)\epsilon(k)$:

$$\epsilon(k) = \left(\epsilon_1^x, \epsilon_1^y, \epsilon_1^z, \epsilon_2^x, \epsilon_2^y, \epsilon_2^z, \cdots \cdots \epsilon_{N_b}^x, \epsilon_{N_b}^y, \epsilon_{N_b}^z\right)$$

- For each atom type, α, we can write:

$$\bar{\epsilon}_\alpha(k) = \left(\epsilon_\alpha^x, \epsilon_\alpha^y, \epsilon_\alpha^z\right)$$

and

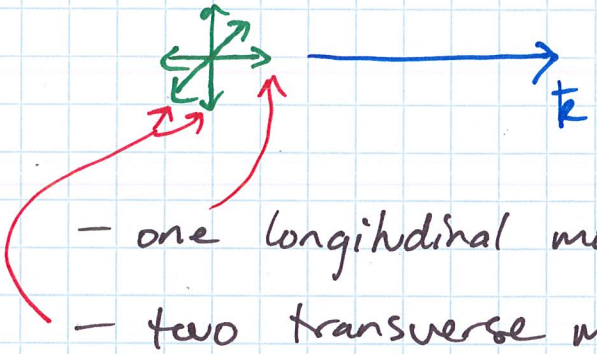
$$\bar{u}_\alpha(n,t) = \frac{\bar{\epsilon}_\alpha(k)}{\sqrt{M_\alpha}} e^{i\bar{k}\cdot(\bar{R}_n^0 + \bar{R}_\alpha^v) - i\omega t}$$

↳ displacement vector

- We see here that $\bar{\epsilon}_\alpha(k)$ represents the "direction" of oscillation, i.e. polarization of the vibrational mode

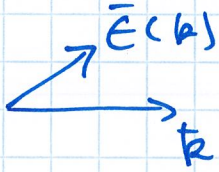
$\bar{\epsilon}_\alpha(k) \rightarrow$ polarization vector

In general, in 3D, oscillations can be $\parallel$ or $\perp$ to k:



- Polarization vector $\bar{\epsilon}(k)$ determines the type of mode

- Although, $\bar{\epsilon}(k)$ need not be exclusively transverse or longitudinal:



(2 - T & L form lin. indep. basis for solutions. Lin. comb. of solutions are also solutions)

- If there are 2 or more atoms in the unit cell, there will be both optical & acoustic modes:

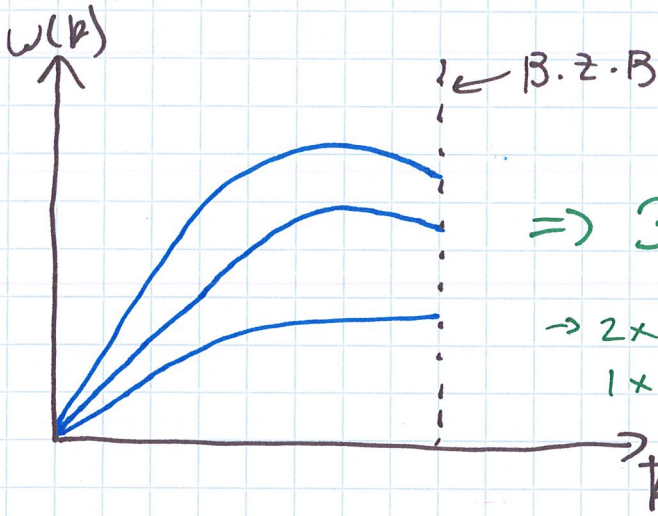
TO : transverse optical

TA : transverse acoustic

LO : longitudinal optical

LA : longitudinal acoustic

e.g. Monatomic 3D solid

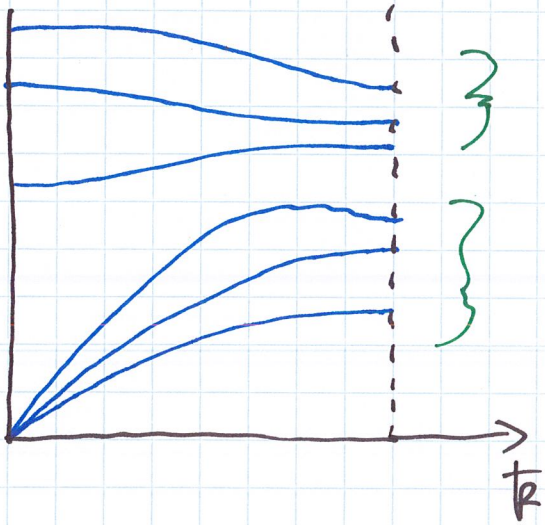


⇒ 3 branches (x, y, z or a_1, a_2, a_3)

→ 2× transverse
1× longitudinal

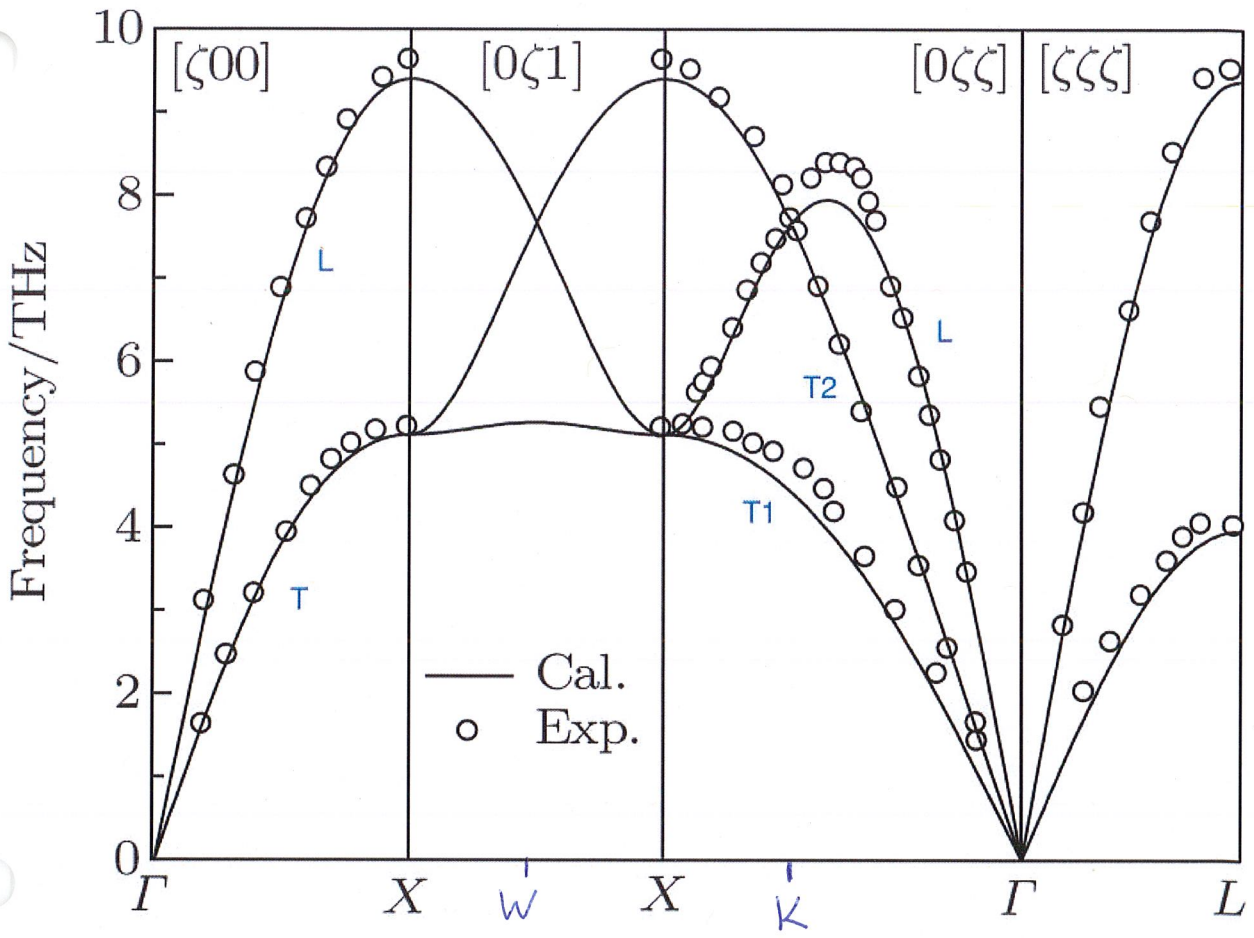
→ of course, depending on the symmetry of the solid, some dispersion curves may be degenerate!

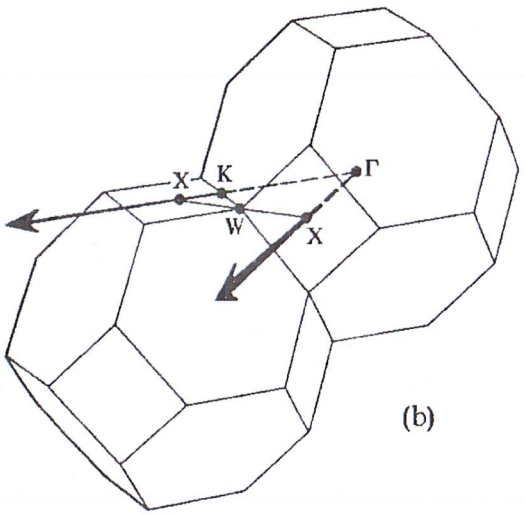
e.g. Diatomic 3D solid



} 3 optical branches (2× TO, 1× LO)

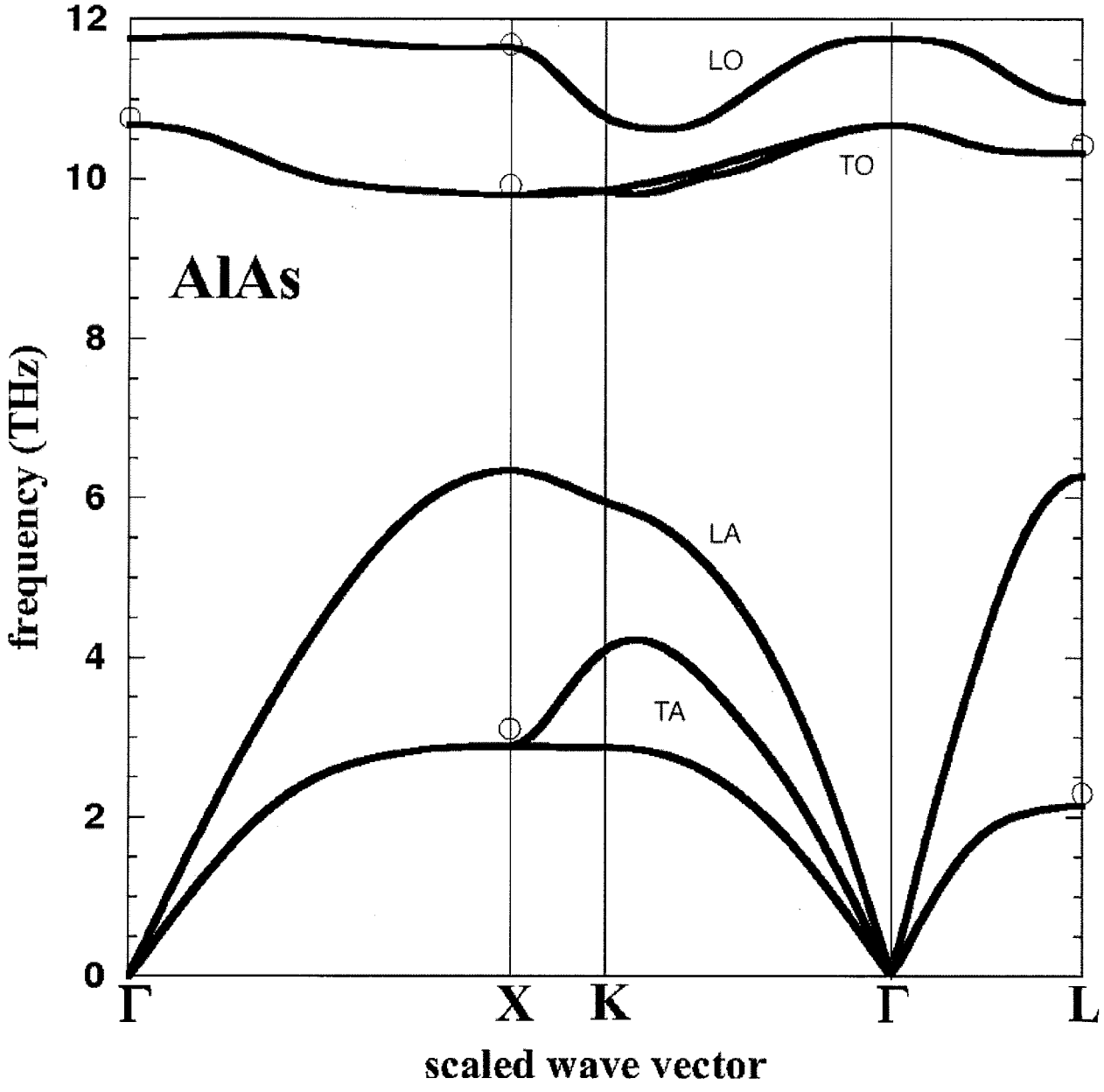
} 3 acoustic branches (2× TA, 1× LA)


Frequency/THz
10
8
6
4
2
0
[ζ00]
[0ζ1]
[0ζζ]
[ζζζ]
L
T
T1
T2
L
Cal.
Exp.
Γ
X
W
X
K
Γ
L

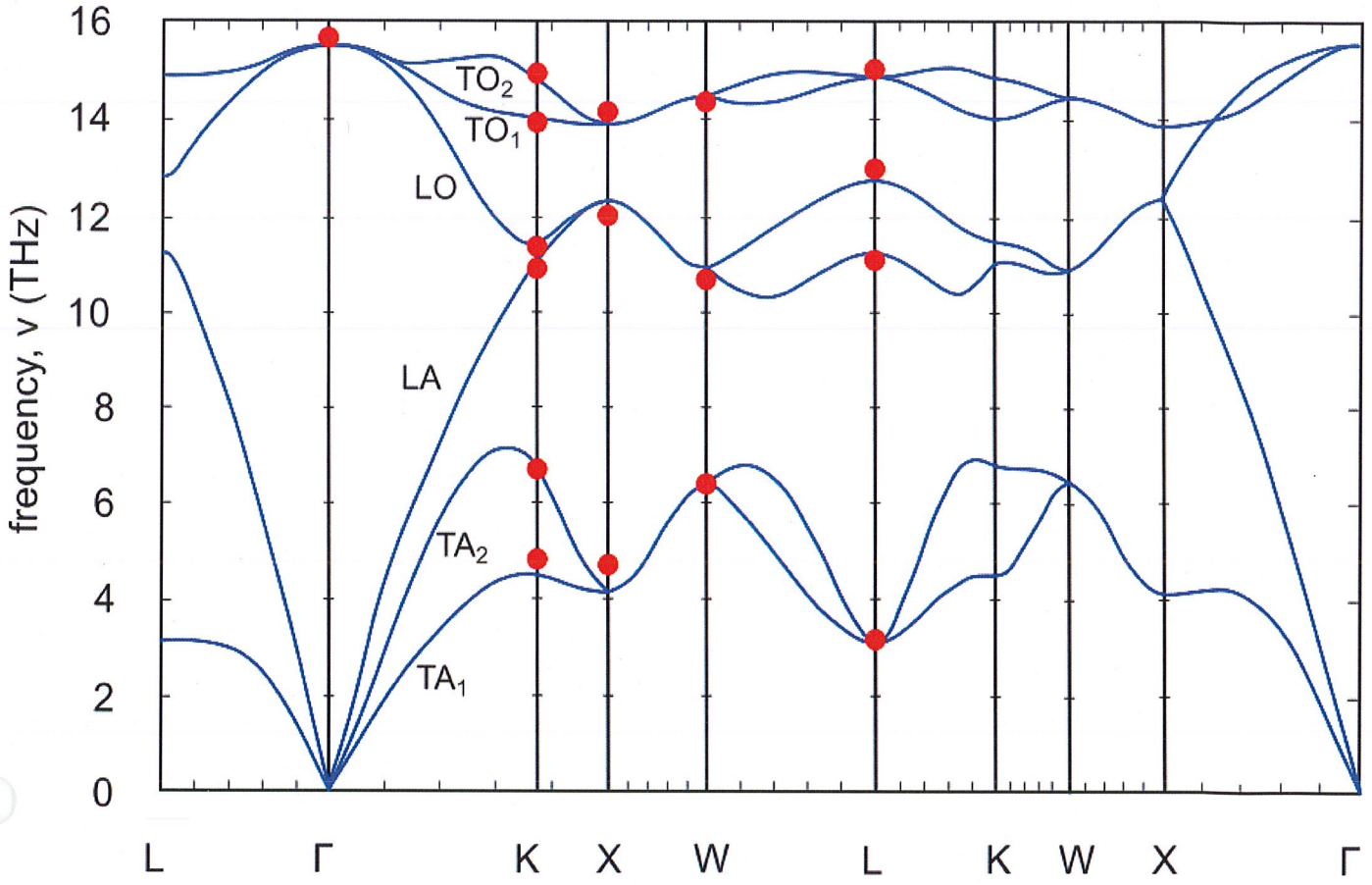

X
K
Γ
W
X

(b)

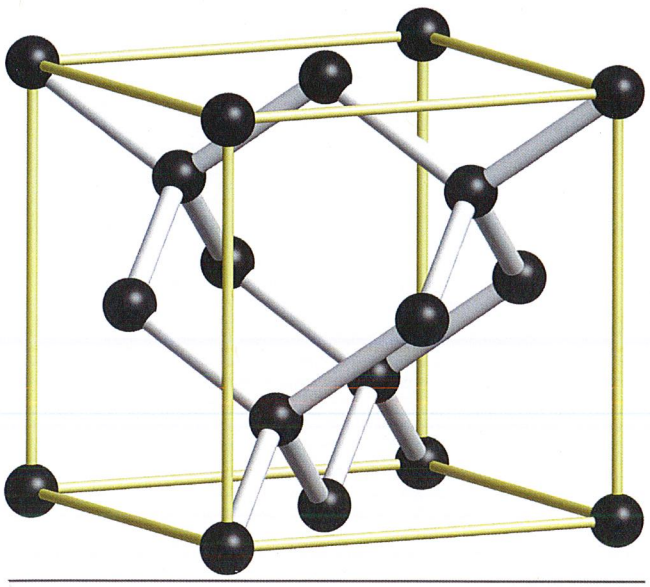
Aluminum


12
10
8
6
4
2
0
frequency (THz)
AlAs
LO
TO
LA
TA
Γ
X
K
Γ
L
scaled wave vector

Silicon (crystalline)



FCC structure, 2-atom basis



2-atom basis

→ Masses equal
$(M_1 = M_2)$

→ Interaction (Force constants) not equal