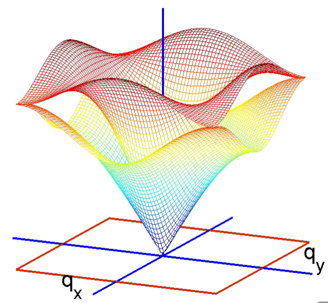
Handout 18

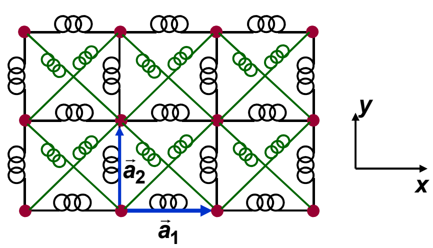
Phonons in 2D Crystals: Monoatomic Basis and Diatomic Basis

In this lecture you will learn:

- Phonons in a 2D crystal with a monoatomic basis
- Phonons in a 2D crystal with a diatomic basis
- Dispersion of phonons
- LA and TA acoustic phonons
- LO and TO optical phonons



Phonons in a 2D Crystal with a Monoatomic Basis



General lattice vector:

$$\vec{R}_{nm} = n\,\vec{a}_1 + m\vec{a}_2$$

Nearest-neighbor vectors:

$$\vec{n}_1 = a\hat{x} \qquad \vec{n}_2 = a\hat{y}$$
$$\vec{n}_3 = -a\hat{x} \qquad \vec{n}_4 = -a\hat{y}$$

Next nearest-neighbor vectors:

$$\vec{p}_1 = a\hat{x} + a\hat{y} \qquad \vec{p}_2 = -a\hat{x} + a\hat{y}$$
$$\vec{p}_3 = -a\hat{x} - a\hat{y} \qquad \vec{p}_4 = a\hat{x} - a\hat{y}$$

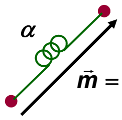
Atomic displacement vectors:

Atoms, can move in 2D therefore atomic displacements are given by a vector:

$$\vec{u}(\vec{R}_{nm},t) = \begin{bmatrix} u_x(\vec{R}_{nm},t) \\ u_y(\vec{R}_{nm},t) \end{bmatrix}$$

Vector Dynamical Equations

$$\vec{u}(\vec{R}_2,t) = \vec{u}(\vec{R}_1 + \vec{m},t)$$



$$\vec{m} = \vec{R}_2 - \vec{R}_1$$

$$\vec{u}(\vec{R}_1,t) \qquad \hat{m} = \frac{\vec{m}}{|\vec{m}|}$$

If the nearest-neighbor vectors are known then the dynamical equations can be written easily.

Vector dynamical equation:

$$M\frac{d^2\vec{u}(\vec{R}_1,t)}{dt^2} = \alpha\left[\left[\vec{u}(\vec{R}_2,t) - \vec{u}(\vec{R}_1,t)\right].\,\hat{m}\right]\hat{m} = \alpha\left[\left[\vec{u}(\vec{R}_1+\vec{m},t) - \vec{u}(\vec{R}_1,t)\right].\,\hat{m}\right]\hat{m}$$

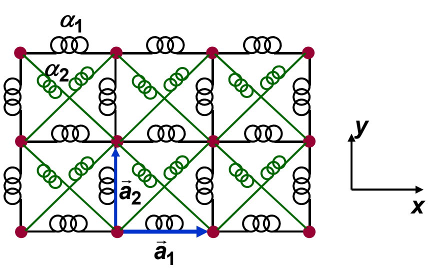
Component dynamical equation:

To find the equations for the x and y-components of the atomic displacement, take the dot-products of the above equation on both sides with $\hat{x}$ and $\hat{y}$, respectively:

$$M\frac{d^2u_x(\vec{R}_1,t)}{dt^2} = \alpha\left[\left[\vec{u}(\vec{R}_1+\vec{m},t) - \vec{u}(\vec{R}_1,t)\right].\,\hat{m}\right](\hat{m}.\hat{x})$$

$$M\frac{d^2u_y(\vec{R}_1,t)}{dt^2} = \alpha\left[\left[\vec{u}(\vec{R}_1+\vec{m},t) - \vec{u}(\vec{R}_1,t)\right].\,\hat{m}\right](\hat{m}.\hat{y})$$

Vector Dynamical Equations for a 2D Crystal



General lattice vector:

$$\vec{R}_{nm} = n\,\vec{a}_1 + m\vec{a}_2$$

Nearest-neighbor vectors:

$\vec{n}_1 = a\hat{x}$ $\qquad \vec{n}_2 = a\hat{y}$

$\vec{n}_3 = -a\hat{x}$ $\qquad \vec{n}_4 = -a\hat{y}$

Next nearest-neighbor vectors:

$\vec{p}_1 = a\hat{x} + a\hat{y}$ $\qquad \vec{p}_2 = -a\hat{x} + a\hat{y}$

$\vec{p}_3 = -a\hat{x} - a\hat{y}$ $\qquad \vec{p}_4 = a\hat{x} - a\hat{y}$

$$M\frac{d^2\vec{u}(\vec{R}_{nm},t)}{dt^2} = \alpha_1 \sum_{j=1,2,3,4}\left[\left[\vec{u}(\vec{R}_{nm}+\vec{n}_j,t) - \vec{u}(\vec{R}_{nm},t)\right].\,\hat{n}_j\right]\hat{n}_j \longrightarrow$$ **summation over 4 nn**

$$+\alpha_2 \sum_{j=1,2,3,4}\left[\left[\vec{u}(\vec{R}_{nm}+\vec{p}_j,t) - \vec{u}(\vec{R}_{nm},t)\right].\,\hat{p}_j\right]\hat{p}_j \longrightarrow$$ **summation over 4 next nn**

Dynamical Equations

$$M\frac{d^2\vec{u}(\vec{R}_{nm},t)}{dt^2} = \alpha_1 \sum_{j=1,2,3,4}\left[\left[\vec{u}(\vec{R}_{nm}+\vec{n}_j,t)-\vec{u}(\vec{R}_{nm},t)\right].\hat{n}_j\right]\hat{n}_j + \alpha_2 \sum_{j=1,2,3,4}\left[\left[\vec{u}(\vec{R}_{nm}+\vec{p}_j,t)-\vec{u}(\vec{R}_{nm},t)\right].\hat{p}_j\right]\hat{p}_j$$

If we take the dot-product of the above equation with $\hat{x}$ we get:

$$\begin{aligned} M\frac{d^2u_x(\vec{R}_{nm},t)}{dt^2} = & -\alpha_1\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{n}_1,t)\right]-\alpha_1\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{n}_3,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_1,t)\right]-\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_1,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_2,t)\right]+\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_2,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_3,t)\right]-\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_3,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_4,t)\right]+\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_4,t)\right] \end{aligned}$$

Dynamical Equations

$$M\frac{d^2\vec{u}(\vec{R}_{nm},t)}{dt^2} = \alpha_1 \sum_{j=1,2,3,4}\left[\left[\vec{u}(\vec{R}_{nm}+\vec{n}_j,t)-\vec{u}(\vec{R}_{nm},t)\right].\hat{n}_j\right]\hat{n}_j + \alpha_2 \sum_{j=1,2,3,4}\left[\left[\vec{u}(\vec{R}_{nm}+\vec{p}_j,t)-\vec{u}(\vec{R}_{nm},t)\right].\hat{p}_j\right]\hat{p}_j$$

If we take the dot-product of the above equation with $\hat{y}$ we get:

$$\begin{aligned} M\frac{d^2u_y(\vec{R}_{nm},t)}{dt^2} = & -\alpha_1\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{n}_2,t)\right]-\alpha_1\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{n}_4,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_1,t)\right]-\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_1,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_2,t)\right]+\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_2,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_3,t)\right]-\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_3,t)\right] \\ & -\frac{\alpha_2}{2}\left[u_y(\vec{R}_{nm},t)-u_y(\vec{R}_{nm}+\vec{p}_4,t)\right]+\frac{\alpha_2}{2}\left[u_x(\vec{R}_{nm},t)-u_x(\vec{R}_{nm}+\vec{p}_4,t)\right] \end{aligned}$$

Solution of the Dynamical Equations

Assume a wave-like solution of the form:

$$\vec{u}(\vec{R}_{nm},t)=\begin{bmatrix}u_x(\vec{R}_{nm},t)\\ u_y(\vec{R}_{nm},t)\end{bmatrix}=\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}e^{i\,\vec{q}\,.\,\vec{R}_{nm}}\;e^{-i\,\omega\,t}$$

Then:

$$\vec{u}(\vec{R}_{nm}+\vec{n}_j,t)=\begin{bmatrix}u_x(\vec{R}_{nm}+\vec{n}_j,t)\\ u_y(\vec{R}_{nm}+\vec{n}_j,t)\end{bmatrix}=\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}e^{i\,\vec{q}\,.\,(\vec{R}_{nm}+\vec{n}_j)}\;e^{-i\,\omega\,t}$$

$$=e^{i\,\vec{q}\,.\,\vec{n}_j}\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}e^{i\,\vec{q}\,.\,\vec{R}_{nm}}\;e^{-i\,\omega\,t}$$

$$=e^{i\,\vec{q}\,.\,\vec{n}_j}\;\vec{u}(\vec{R}_{nm},t)$$

We take the above solution form and plug it into the dynamical equations

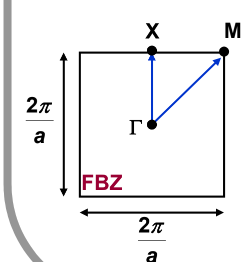
Dynamical Matrix and Phonon Bands

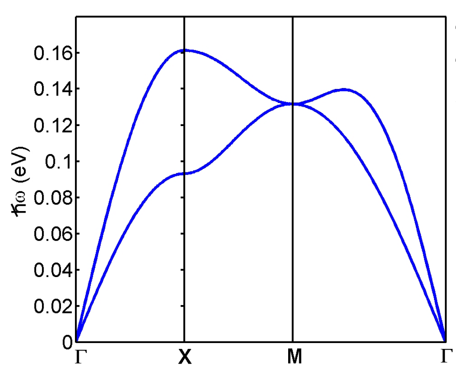
$$\begin{bmatrix}4\alpha_1\sin^2\left(\frac{q_x a}{2}\right)+2\alpha_2\left[1-\cos(q_x a)\cos(q_y a)\right] & 2\alpha_2\sin(q_x a)\sin(q_y a)\\ 2\alpha_2\sin(q_x a)\sin(q_y a) & 4\alpha_1\sin^2\left(\frac{q_y a}{2}\right)+2\alpha_2\left[1-\cos(q_x a)\cos(q_y a)\right]\end{bmatrix}\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}=\omega^2 M\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}$$

Compare with the standard form:

$$\overline{\overline{D}}(\vec{q})\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}=\omega^2\begin{bmatrix}M & 0\\ 0 & M\end{bmatrix}\begin{bmatrix}u_x(\vec{q})\\ u_y(\vec{q})\end{bmatrix}$$

Solutions:





$\alpha_1 = 200$ N/m

$\alpha_2 = 100$ N/m

$M = 2\text{x}10^{-26}$ kg

Transverse (TA) and Longitudinal (LA) Acoustic Phonons

$$\begin{bmatrix} 4\alpha_1\left(\frac{q_x a}{2}\right)^2 + \alpha_2\left[(q_x a)^2 + (q_y a)^2\right] & 2\alpha_2(q_x a)(q_y a) \\ 2\alpha_2(q_x a)(q_y a) & 4\alpha_1\left(\frac{q_y a}{2}\right)^2 + \alpha_2\left[(q_x a)^2 + (q_y a)^2\right] \end{bmatrix} \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = \omega^2 M \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix}$$

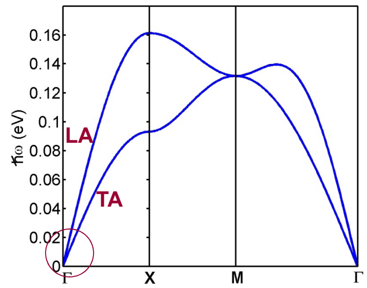
Case I: $q_x \approx 0 \, , q_y = 0$

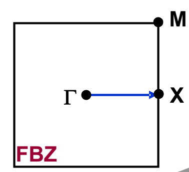
$$\omega_{LA}(q_x) = \sqrt{\frac{\alpha_1 + \alpha_2}{M}} \, q_x a \qquad \begin{bmatrix} u_x(q_x) \\ u_y(q_x) \end{bmatrix} = A \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Longitudinal acoustic phonons: atomic motion in the direction of wave propagation

$$\omega_{TA}(q_x) = \sqrt{\frac{\alpha_2}{M}} \, q_x a \qquad \begin{bmatrix} u_x(q_x) \\ u_y(q_x) \end{bmatrix} = A \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Transverse acoustic phonons: atomic motion in the direction perpendicular to wave propagation





Transverse (TA) and Longitudinal (LA) Acoustic Phonons

$$\begin{bmatrix} 4\alpha_1\left(\frac{q_x a}{2}\right)^2 + \alpha_2\left[(q_x a)^2 + (q_y a)^2\right] & 2\alpha_2(q_x a)(q_y a) \\ 2\alpha_2(q_x a)(q_y a) & 4\alpha_1\left(\frac{q_y a}{2}\right)^2 + \alpha_2\left[(q_x a)^2 + (q_y a)^2\right] \end{bmatrix} \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = \omega^2 M \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix}$$

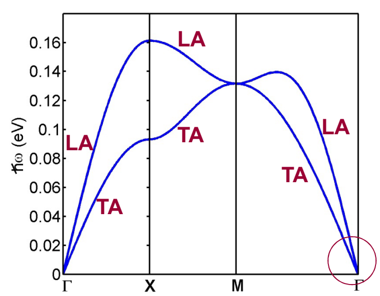
Case II: $q_x \approx 0 \, , q_y \approx 0 \qquad q_x = q_y = q$

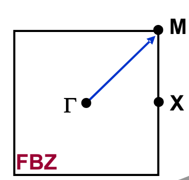
$$\omega_{LA}(q) = \sqrt{\frac{\alpha_1 + 4\alpha_2}{M}} \, q \, a \qquad \begin{bmatrix} u_x(q) \\ u_y(q) \end{bmatrix} = A \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Longitudinal acoustic phonons: atomic motion in the direction of wave propagation

$$\omega_{TA}(q) = \sqrt{\frac{\alpha_1}{M}} \, q \, a \qquad \begin{bmatrix} u_x(q) \\ u_y(q) \end{bmatrix} = A \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Transverse acoustic phonons: atomic motion in the direction perpendicular to wave propagation





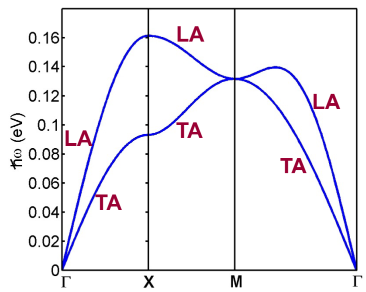
Transverse (TA) and Longitudinal (LA) Acoustic Phonons

In general for longitudinal acoustic phonons near the zone center:

$$\begin{bmatrix} u_x(q) \\ u_y(q) \end{bmatrix} = \frac{A}{|\vec{q}|} \begin{bmatrix} q_x \\ q_y \end{bmatrix}$$

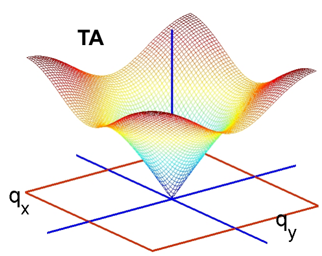
And for transverse acoustic phonons near the zone center:

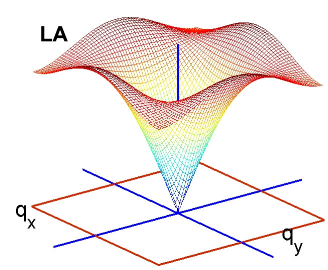
$$\begin{bmatrix} u_x(q) \\ u_y(q) \end{bmatrix} = \frac{A}{|\vec{q}|} \begin{bmatrix} -q_y \\ q_x \end{bmatrix}$$

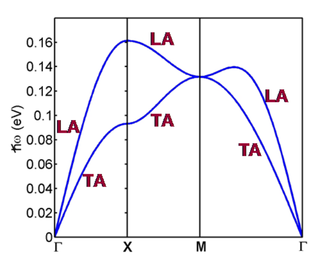


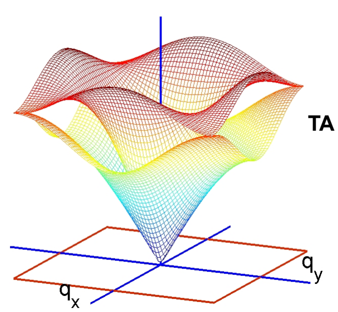
In general, away from the zone center, the LA phonons are not entirely longitudinal and neither the TA phonons are entirely transverse

Transverse (TA) and Longitudinal (LA) Acoustic Phonons









Periodic Boundary Conditions in 2D

General lattice vector:

$$\vec{R}_{nm} = n\,\vec{a}_1 + m\vec{a}_2$$

General reciprocal lattice vector inside FBZ:

$$\vec{q} = \alpha_1\,\vec{b}_1 + \alpha_2\,\vec{b}_2 \qquad \{ \quad -1/2 \le \alpha_1\,,\alpha_2 \le 1/2$$

Our solution was:

$$\vec{u}(\vec{R}_{nm},t) = \begin{bmatrix} u_x(\vec{R}_{nm},t) \\ u_y(\vec{R}_{nm},t) \end{bmatrix} = \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} e^{i\,\vec{q}\,.\,\vec{R}_{nm}}\; e^{-i\,\omega\,t}$$

Periodic boundary conditions for a lattice of N_1xN_2 primitive cells imply:

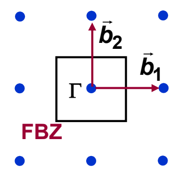
$$\vec{u}(\vec{R}_{nm} + N_1\vec{a}_1, t) = \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} e^{i\,\vec{q}\,.\,(\vec{R}_{nm}+N_1\vec{a}_1)}\; e^{-i\,\omega\,t} = \vec{u}(\vec{R}_{nm},t) = \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} e^{i\,\vec{q}\,.\,\vec{R}_{nm}}\; e^{-i\,\omega\,t}$$

$$\Rightarrow e^{i\,\vec{q}\,.\,N_1\vec{a}_1} = 1$$

$$\Rightarrow \vec{q}\,.\,N_1\vec{a}_1 = m_1\,2\pi \qquad \{\text{ where } m_1 \text{ is an integer}$$

$$\Rightarrow 2\pi\,\alpha_1\,N_1 = m_1\,2\pi \qquad \left\{ \text{ where } -\frac{1}{2} < \alpha_1 \le \frac{1}{2} \right.$$

$$\Rightarrow \alpha_1 = \frac{m_1}{N_1} \qquad \left\{ \text{ where } -\frac{N_1}{2} < m \le \frac{N_1}{2} \right.$$



Similarly:

$$\alpha_2 = \frac{m_2}{N_2} \qquad \left\{ \text{ where } -\frac{N_2}{2} < m_2 \le \frac{N_2}{2} \right.$$

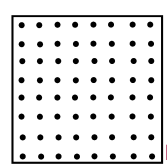
Counting Degrees of Freedom

In the solution the values of the phonon wavevector are dictated by the periodic boundary conditions:

$$\vec{q} = \alpha_1\,\vec{b}_1 + \alpha_2\,\vec{b}_2$$

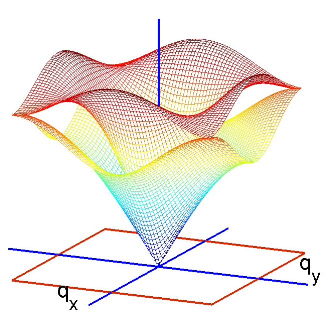
$$\alpha_1 = \frac{m_1}{N_1} \qquad \left\{ \text{ where } -\frac{N_1}{2} < m \le \frac{N_1}{2} \right.$$

$$\alpha_2 = \frac{m_2}{N_2} \qquad \left\{ \text{ where } -\frac{N_2}{2} < m_2 \le \frac{N_2}{2} \right.$$



$\Rightarrow$There are N_1N_2 allowed wavevectors in the FBZ (There are also N_1N_2 primitive cells in the crystals)

$\Rightarrow$There are N_1N_2 phonon modes per phonon band



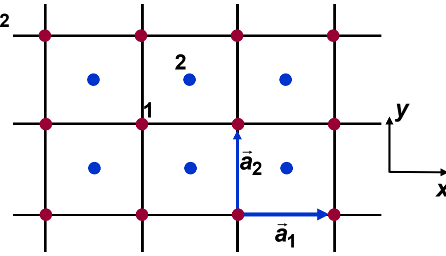
Counting degrees of freedom:

- There are $2N_1N_2$ degrees of freedom corresponding to the motion in 2D of N_1N_2 atoms

- The total number of different phonon modes in the two bands is also $2N_1N_2$

Phonons in a 2D Crystal with a Diatomic Basis

$$\vec{R}_{nm} = n\,\vec{a}_1 + m\vec{a}_2$$



Atomic displacement vectors:

The two atoms in a primitive cell can move in 2D therefore atomic displacements are given by a four-component column vector:

$$\begin{bmatrix} \vec{u}_1(\vec{R}_{nm} + \vec{d}_1, t) \\ \vec{u}_2(\vec{R}_{nm} + \vec{d}_2, t) \end{bmatrix} = \begin{bmatrix} u_{1x}(\vec{R}_{nm} + \vec{d}_1, t) \\ u_{1y}(\vec{R}_{nm} + \vec{d}_1, t) \\ u_{2x}(\vec{R}_{nm} + \vec{d}_2, t) \\ u_{2y}(\vec{R}_{nm} + \vec{d}_2, t) \end{bmatrix}$$

1st nearest-neighbor vectors (red to blue):

$$\vec{h}_1 = \frac{a\hat{x} + a\hat{y}}{2} \qquad \vec{h}_2 = \frac{-a\hat{x} + a\hat{y}}{2}$$

$$\vec{h}_3 = \frac{-a\hat{x} - a\hat{y}}{2} \qquad \vec{h}_4 = \frac{a\hat{x} - a\hat{y}}{2}$$

2nd nearest-neighbor vectors (red to red):

$$\vec{n}_1 = a\hat{x} \qquad \vec{n}_2 = a\hat{y}$$

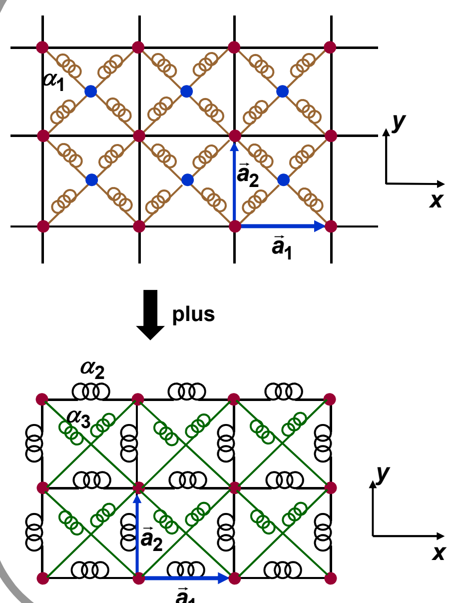
$$\vec{n}_3 = -a\hat{x} \qquad \vec{n}_4 = -a\hat{y}$$

3rd nearest-neighbor vectors (red to red):

$$\vec{p}_1 = a\hat{x} + a\hat{y} \qquad \vec{p}_2 = -a\hat{x} + a\hat{y}$$

$$\vec{p}_3 = -a\hat{x} - a\hat{y} \qquad \vec{p}_4 = a\hat{x} - a\hat{y}$$

Diatomic Basis: Force Constants



The force constants between the 1st 2nd and 3rd nearest-neighbors need to be included (at least)

Diatomic Basis: Dynamical Equations

Dynamical equation for the red(1) atom:

$$M_1 \frac{d^2\vec{u}_1(\vec{R}_{nm}+\vec{d}_1,t)}{dt^2} = +\alpha_1 \sum_{j=1,2,3,4}\left[\left[\vec{u}_2(\vec{R}_{nm}+\vec{d}_1+\vec{h}_j,t)-\vec{u}_1(\vec{R}_{nm}+\vec{d}_1,t)\right].\hat{h}_j\right]\hat{h}_j \longrightarrow \text{summation over 4 1}^{st}\text{ nn}$$

$$+\alpha_2 \sum_{j=1,2,3,4}\left[\left[\vec{u}_1(\vec{R}_{nm}+\vec{d}_1+\vec{n}_j,t)-\vec{u}_1(\vec{R}_{nm}+\vec{d}_1,t)\right].\hat{n}_j\right]\hat{n}_j \longrightarrow \text{summation over 4 2}^{nd}\text{ nn}$$

$$+\alpha_3 \sum_{j=1,2,3,4}\left[\left[\vec{u}_1(\vec{R}_{nm}+\vec{d}_1+\vec{p}_j,t)-\vec{u}_1(\vec{R}_{nm}+\vec{d}_1,t)\right].\hat{p}_j\right]\hat{p}_j \longrightarrow \text{summation over 4 3}^{rd}\text{ nn}$$

Dynamical equation for the blue(2) atom:

$$M_2 \frac{d^2\vec{u}_2(\vec{R}_{nm}+\vec{d}_2,t)}{dt^2} = +\alpha_1 \sum_{j=1,2,3,4}\left[\left[\vec{u}_2(\vec{R}_{nm}+\vec{d}_2+\vec{h}_j,t)-\vec{u}_2(\vec{R}_{nm}+\vec{d}_2,t)\right].\hat{h}_j\right]\hat{h}_j \longrightarrow \text{summation over 4 1}^{st}\text{ nn}$$

$$+\alpha_2 \sum_{j=1,2,3,4}\left[\left[\vec{u}_2(\vec{R}_{nm}+\vec{d}_2+\vec{n}_j,t)-\vec{u}_2(\vec{R}_{nm}+\vec{d}_2,t)\right].\hat{n}_j\right]\hat{n}_j \longrightarrow \text{summation over 4 2}^{nd}\text{ nn}$$

$$+\alpha_3 \sum_{j=1,2,3,4}\left[\left[\vec{u}_2(\vec{R}_{nm}+\vec{d}_2+\vec{p}_j,t)-\vec{u}_2(\vec{R}_{nm}+\vec{d}_2,t)\right].\hat{p}_j\right]\hat{p}_j \longrightarrow \text{summation over 4 3}^{rd}\text{ nn}$$

Diatomic Basis: Dynamical Equations

Assume a solution of the form:

$$\begin{bmatrix}\vec{u}_1(\vec{R}_{nm}+\vec{d}_1,t)\\ \vec{u}_2(\vec{R}_{nm}+\vec{d}_2,t)\end{bmatrix} = \begin{bmatrix}u_{1x}(\vec{R}_{nm}+\vec{d}_1,t)\\ u_{1y}(\vec{R}_{nm}+\vec{d}_1,t)\\ u_{2x}(\vec{R}_{nm}+\vec{d}_2,t)\\ u_{2y}(\vec{R}_{nm}+\vec{d}_2,t)\end{bmatrix} = \begin{bmatrix}u_{1x}(\vec{q})\,e^{i\,\vec{q}\,.\,\vec{d}_1}\\ u_{1y}(\vec{q})e^{i\,\vec{q}\,.\,\vec{d}_1}\\ u_{2x}(\vec{q})e^{i\,\vec{q}\,.\,\vec{d}_2}\\ u_{2y}(\vec{q})e^{i\,\vec{q}\,.\,\vec{d}_2}\end{bmatrix} e^{i\,\vec{q}\,.\,\vec{R}_{nm}}\; e^{-i\,\omega\,t}$$

To get a matrix equation of the form:

$$\overline{\overline{D}}(\vec{q})\begin{bmatrix}u_{1x}(\vec{q})\\ u_{1y}(\vec{q})\\ u_{2x}(\vec{q})\\ u_{2y}(\vec{q})\end{bmatrix} = \omega^2\begin{bmatrix}M_1 & 0 & 0 & 0\\ 0 & M_1 & 0 & 0\\ 0 & 0 & M_2 & 0\\ 0 & 0 & 0 & M_2\end{bmatrix}\begin{bmatrix}u_{1x}(\vec{q})\\ u_{1y}(\vec{q})\\ u_{2x}(\vec{q})\\ u_{2y}(\vec{q})\end{bmatrix}$$

The Dynamical Matrix

$$\overline{\overline{D}}(\vec{q})\begin{bmatrix} u_{1x}(\vec{q}) \\ u_{1y}(\vec{q}) \\ u_{2x}(\vec{q}) \\ u_{2y}(\vec{q}) \end{bmatrix} = \omega^2 \begin{bmatrix} M_1 & 0 & 0 & 0 \\ 0 & M_1 & 0 & 0 \\ 0 & 0 & M_2 & 0 \\ 0 & 0 & 0 & M_2 \end{bmatrix}\begin{bmatrix} u_{1x}(\vec{q}) \\ u_{1y}(\vec{q}) \\ u_{2x}(\vec{q}) \\ u_{2y}(\vec{q}) \end{bmatrix}$$

The matrix $\overline{\overline{D}}(\vec{q})$ is:

$2\alpha_1 + 4\alpha_2 \sin^2\left(\frac{q_x a}{2}\right) + 2\alpha_3\left[1-\cos(q_x a)\cos(q_y a)\right]$	$2\alpha_3 \sin(q_x a)\sin(q_y a)$	$-2\alpha_1 \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)$	$2\alpha_1 \sin\left(\frac{q_x a}{2}\right)\sin\left(\frac{q_y a}{2}\right)$
$2\alpha_3 \sin(q_x a)\sin(q_y a)$	$2\alpha_1 + 4\alpha_2 \sin^2\left(\frac{q_y a}{2}\right) + 2\alpha_3\left[1-\cos(q_x a)\cos(q_y a)\right]$	$2\alpha_1 \sin\left(\frac{q_x a}{2}\right)\sin\left(\frac{q_y a}{2}\right)$	$-2\alpha_1 \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)$
$-2\alpha_1 \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)$	$2\alpha_1 \sin\left(\frac{q_x a}{2}\right)\sin\left(\frac{q_y a}{2}\right)$	$2\alpha_1 + 4\alpha_2 \sin^2\left(\frac{q_x a}{2}\right) + 2\alpha_3\left[1-\cos(q_x a)\cos(q_y a)\right]$	$2\alpha_3 \sin(q_x a)\sin(q_y a)$
$2\alpha_1 \sin\left(\frac{q_x a}{2}\right)\sin\left(\frac{q_y a}{2}\right)$	$-2\alpha_1 \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)$	$2\alpha_3 \sin(q_x a)\sin(q_y a)$	$2\alpha_1 + 4\alpha_2 \sin^2\left(\frac{q_y a}{2}\right) + 2\alpha_3\left[1-\cos(q_x a)\cos(q_y a)\right]$

Diatomic Basis: Solution and Phonon Bands

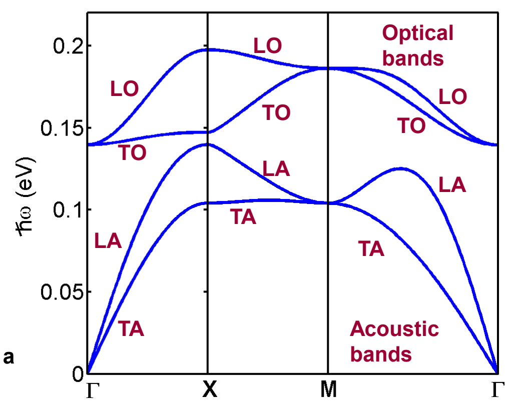
For calculations:

$2M_1 = M_2 = 4\times10^{-26}$ kg

$\alpha_1 = 300$ N/m

$\alpha_2 = 200$ N/m

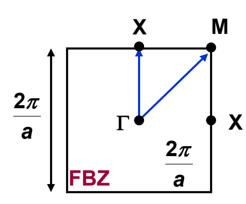
$\alpha_3 = 100$ N/m



One obtains:

- 2 optical phonon bands (that have a non-zero frequency at the zone center)

- 2 acoustic phonon bands (that have zero frequency at the zone center)



Longitudinal (LO) and Transverse (TO) Optical Phonons

Case I: $q_x \approx 0\,,\, q_y = 0$

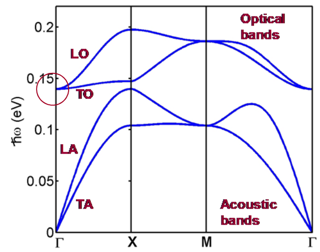
$$\frac{1}{M_r} = \frac{1}{M_1} + \frac{1}{M_2}$$

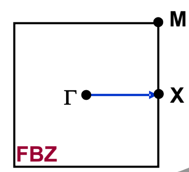
$$\omega_{LO}(q_x \approx 0) = \sqrt{\frac{2\alpha_1}{M_r}} \qquad \begin{bmatrix} u_{1x}(q_x) \\ u_{1y}(q_x) \\ u_{2x}(q_x) \\ u_{2y}(q_x) \end{bmatrix} = A \begin{bmatrix} 1 \\ 0 \\ -M_1/M_2 \\ 0 \end{bmatrix}$$

Longitudinal optical phonons: atomic motion in the direction of wave propagation and basis atoms move out of phase

$$\omega_{TO}(q_x \approx 0) = \sqrt{\frac{2\alpha_1}{M_r}} \qquad \begin{bmatrix} u_{1x}(q_x) \\ u_{1y}(q_x) \\ u_{2x}(q_x) \\ u_{2y}(q_x) \end{bmatrix} = A \begin{bmatrix} 0 \\ 1 \\ 0 \\ -M_1/M_2 \end{bmatrix}$$

Transverse optical phonons: atomic motion in the direction perpendicular to wave propagation and basis atoms move out of phase





Longitudinal (LA) and Transverse (TA) Acoustic Phonons

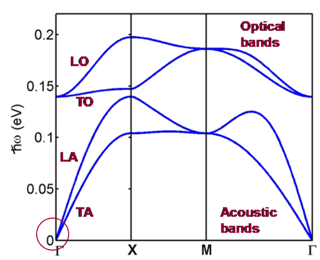
Case I: $q_x \approx 0\,,\, q_y = 0$

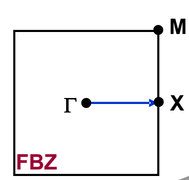
$$\omega_{LA}(q_x \approx 0) = ? \qquad \begin{bmatrix} u_{1x}(q_x) \\ u_{1y}(q_x) \\ u_{2x}(q_x) \\ u_{2y}(q_x) \end{bmatrix} = A \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

Longitudinal acoustic phonons: atomic motion in the direction of wave propagation and basis atoms move in phase

$$\omega_{TO}(q_x \approx 0) = ? \qquad \begin{bmatrix} u_{1x}(q_x) \\ u_{1y}(q_x) \\ u_{2x}(q_x) \\ u_{2y}(q_x) \end{bmatrix} = A \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

Transverse acoustic phonons: atomic motion in the direction perpendicular to wave propagation and basis atoms move in phase





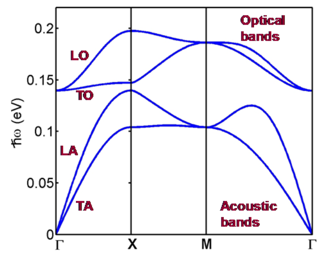
Counting Degrees of Freedom and the Number of Phonon Bands

Periodic boundary conditions for a lattice of N_1xN_2 primitive cells imply:

$$\vec{q} = \alpha_1 \vec{b}_1 + \alpha_2 \vec{b}_2$$

$$\alpha_1 = \frac{m_1}{N_1} \quad \left\{ \text{where } -\frac{N_1}{2} < m \le \frac{N_1}{2} \right.$$

$$\alpha_2 = \frac{m_2}{N_2} \quad \left\{ \text{where } -\frac{N_2}{2} < m_2 \le \frac{N_2}{2} \right.$$



⇒There are N_1N_2 allowed wavevectors in the FBZ
⇒There are N_1N_2 phonon modes per phonon band

Counting degrees of freedom:

• There are $4N_1N_2$ degrees of freedom corresponding to the motion in 2D of $2N_1N_2$ atoms (2 atoms in each primitive cell)

• The total number of different phonon modes in the four bands is also $4N_1N_2$