Handout 19

Lattice Waves (Phonons) in 3D Crystals
Group IV and Group III-V Semiconductors
LO and TO Phonons in Polar Crystals
and
Macroscopic Models of Acoustic Phonons in Solids

In this lecture you will learn:

- Lattice waves (phonons) in 3D crystals
- Phonon bands in group IV and group III-V Semiconductors

- Macroscopic description of acoustic phonons from elasticity theory
- Stress, strain, and Hooke's law

Counting the Number of Phonon bands in 3D Crystals

Periodic boundary conditions for a lattice of $N_1 x N_2 x N_3$ primitive cells imply:

$$\vec{q} = \alpha_1 \vec{b}_1 + \alpha_2 \vec{b}_2 + \alpha_3 \vec{b}_3$$

$$\alpha_1 = m_1/N_1 \quad \{\text{where } -N_1/2 < m_1 \leq N_1/2$$

$$\alpha_2 = m_2/N_2 \quad \{\text{where } -N_2/2 < m_2 \leq N_2/2$$

$$\alpha_3 = m_3/N_3 \quad \{\text{where } -N_3/2 < m_3 \leq N_3/2$$

⇒There are $N_1N_2N_3$ allowed wavevectors in the FBZ
⇒There are $N_1N_2N_3$ phonon modes per phonon band

Counting degrees of freedom and the number of phonon bands: Monoatomic Basis

- There are $3N_1N_2N_3$ degrees of freedom corresponding to the motion in 3D of $N_1N_2N_3$ atoms

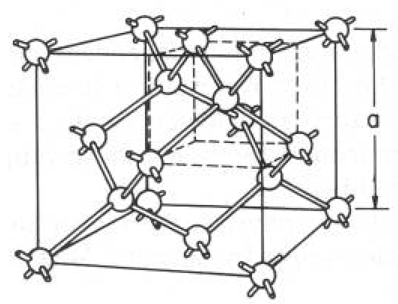
⇒The number of phonon bands must be 3 (two TA bands and one LA band)

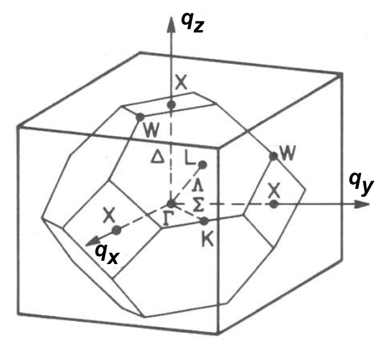
Counting degrees of freedom and the number of phonon bands: Diatomic Basis

- There are $6N_1N_2N_3$ degrees of freedom corresponding to the motion in 3D of $2N_1N_2N_3$ atoms

⇒The number of phonon bands must be 6 (two TA bands and one LA band for acoustic phonons and two TO bands and one LO band for optical phonons)

Phonon Bands in Silicon



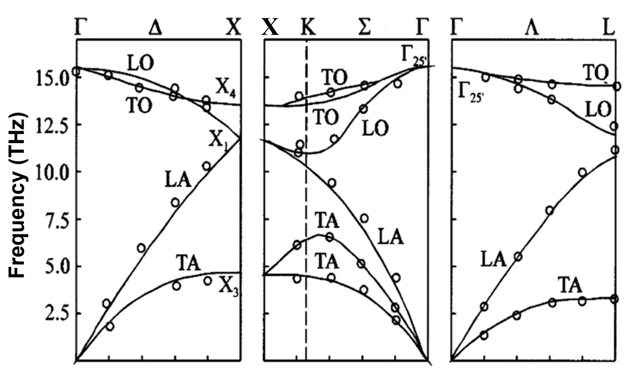


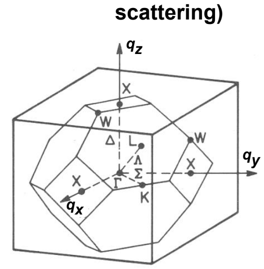
Silicon has a FCC lattice with two basis atoms in one primitive cell

FBZ of Silicon

⇒The number of phonon bands must be 6; two TA bands and one LA band for acoustic phonons and two TO bands and one LO band for optical phonons

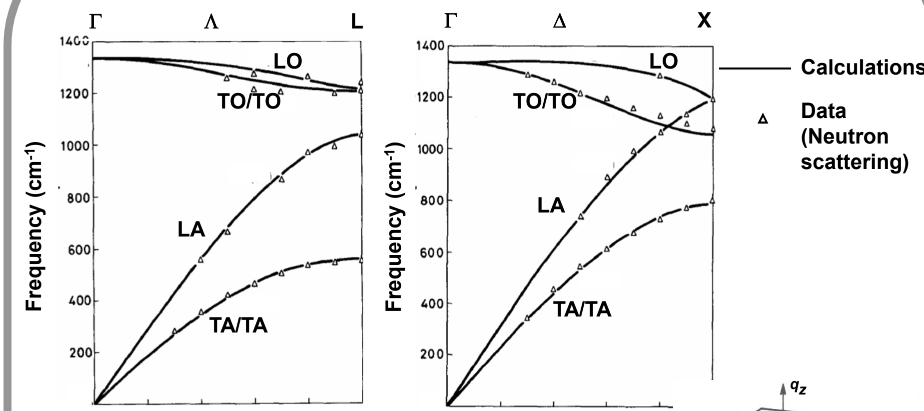
Phonon Bands in Silicon

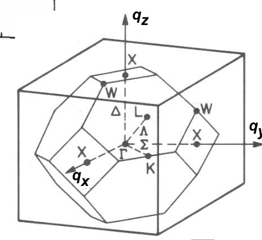




$$\hbar\omega_{LO}(q_x \approx 0) = \hbar\omega_{TO}(q_x \approx 0) = 64 \text{ meV}$$

Phonon Bands in Diamond



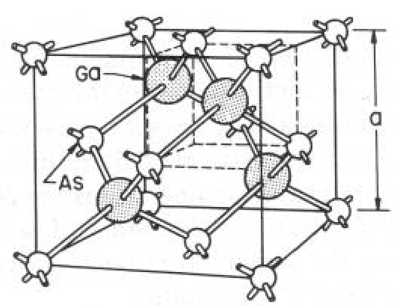


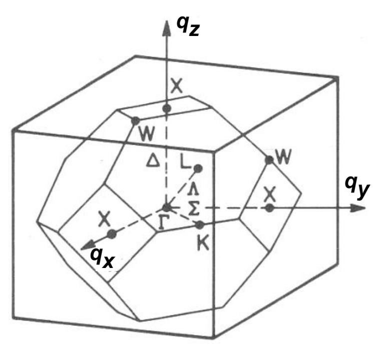
$\hbar\omega_{LO}(q_x \approx 0) = \hbar\omega_{TO}(q_x \approx 0) = 165$ meV   Large!!

Phonon frequencies are also expressed in units of equivalent photon wavelength inverse:

$$\frac{\omega_{LO}(q_x \approx 0)}{2\pi c} = \frac{\omega_{TO}(q_x \approx 0)}{2\pi c} = 1330 \text{ cm}^{-1}$$

Phonon Bands in GaAs



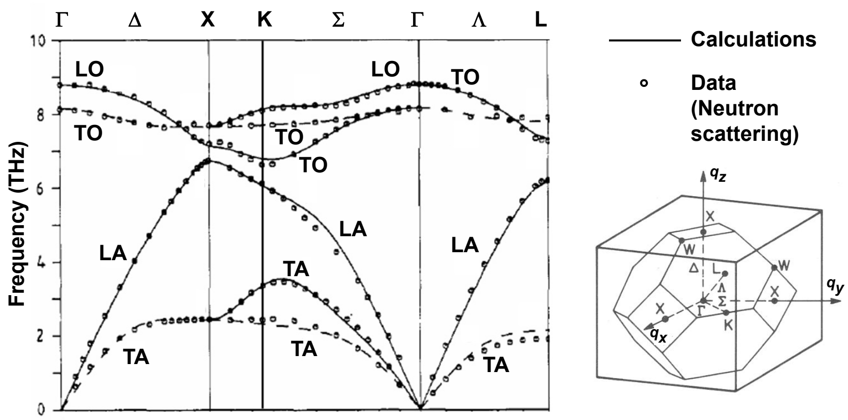


GaAs has a FCC lattice with two basis atoms in one primitive cell

FBZ of GaAs

⇒The number of phonon bands must be 6; two TA bands and one LA band for acoustic phonons and two TO bands and one LO band for optical phonons

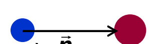
Phonon Bands in GaAs



$$\hbar\omega_{LO}(q_x \approx 0) = 36\ \text{meV}$$
$$\hbar\omega_{TO}(q_x \approx 0) = 33\ \text{meV}$$

Optical Phonons in Polar Crystals

Consider a crystal, like GaAs, made up of two different kind of atoms with a polar covalent bond



$$\vec{u}_1(\vec{R}+\vec{d}_1,t) \quad \vec{n}_j \quad \vec{u}_2(\vec{R}+\vec{d}_1+\vec{n}_j,t)$$

When the atoms move, an oscillating charge dipole is created with a dipole moment given by:

$$\vec{p}_j(\vec{R},t) = f\left[\vec{u}_2(\vec{R}+\vec{d}_1+\vec{n}_j,t) - \vec{u}_1(\vec{R}+\vec{d}_1,t)\right]$$

The material polarization, or the dipole moment density, is then:

$$\vec{P}(\vec{R},t) = \frac{n}{Z}\sum_j \vec{p}_j(\vec{R},t) = \frac{nf}{Z}\sum_j\left[\vec{u}_2(\vec{R}+\vec{d}_1+\vec{n}_j,t) - \vec{u}_1(\vec{R}+\vec{d}_1,t)\right]$$

where:

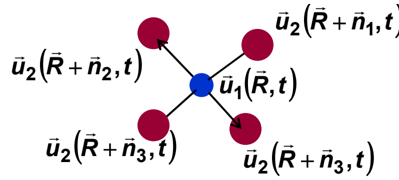
$$n = \frac{1}{\Omega_3} = \text{Number of primitive cells per unit volume}$$

$$Z = \text{Number of nearest neighbors}$$

A non-zero polarization means an electric field!

Optical Phonons in Polar Crystals: D-Field and E-Field

A non-zero polarization means an electric field! How do we find it?



The divergence of the D-field is zero inside the crystal:

$$\nabla.\vec{D} = \rho_u = 0$$

But inside the crystal:

$$\vec{D} = \varepsilon(\infty)\vec{E} + \vec{P}$$

$$\Rightarrow \nabla.\vec{E} = -\frac{\nabla.\vec{P}}{\varepsilon(\infty)}$$

Since:

$$\vec{P}(\vec{R},t) = \frac{n}{Z}\sum_j \vec{p}_j(\vec{R},t) = \frac{nf}{Z}\sum_j \left[\vec{u}_2(\vec{R}+\vec{d}_1+\vec{n}_j,t) - \vec{u}_1(\vec{R}+\vec{d}_1,t)\right]$$

Therefore:

$$\nabla.\vec{E}(\vec{R},t) = -\frac{\nabla.\vec{P}(\vec{R},t)}{\varepsilon(\infty)} \longrightarrow$$

We must also have:

$$\nabla\times\vec{E}(\vec{R},t) = 0$$

Optical Phonons in Polar Crystals: Dynamical Equations

Dynamical equations (assuming only nearest neighbor interactions):

$$\frac{d^2\vec{u}_1(\vec{R}+\vec{d}_1,t)}{dt^2} = \frac{\alpha}{M_1}\sum_j \left[\left[\vec{u}_2(\vec{R}+\vec{d}_1+\vec{n}_j,t) - \vec{u}_1(\vec{R}+\vec{d}_1,t)\right].\hat{n}_j\right]\hat{n}_j - \frac{f}{M_1}\vec{E}(\vec{R},t)$$

$$\frac{d^2\vec{u}_2(\vec{R}+\vec{d}_2,t)}{dt^2} = -\frac{\alpha}{M_2}\sum_j \left[\left[\vec{u}_2(\vec{R}+\vec{d}_2,t) - \vec{u}_1(\vec{R}+\vec{d}_2-\vec{n}_j,t)\right].\hat{n}_j\right]\hat{n}_j + \frac{f}{M_2}\vec{E}(\vec{R},t)$$

Suppose:

$$\begin{bmatrix}\vec{u}_1(\vec{R}+\vec{d}_1,t)\\ \vec{u}_2(\vec{R}+\vec{d}_2,t)\end{bmatrix} = \begin{bmatrix}\vec{u}_1(\vec{q})e^{i\vec{q}.\vec{d}_1}\\ \vec{u}_2(\vec{q})e^{i\vec{q}.\vec{d}_2}\end{bmatrix} e^{i\vec{q}.\vec{R}-i\omega t} \qquad \begin{aligned}\vec{E}(\vec{R},t) &= \vec{E}(\vec{q})\,e^{i\vec{q}.\vec{R}-i\omega t}\\ \vec{P}(\vec{R},t) &= \vec{P}(\vec{q})\,e^{i\vec{q}.\vec{R}-i\omega t}\end{aligned}$$

We have:

$$\nabla\times\vec{E}(\vec{R},t) = 0 \quad\Rightarrow\quad \vec{q}\times\vec{E}(\vec{q}) = 0$$

We also have:

$$\nabla.\vec{E}(\vec{R},t) = -\frac{\nabla.\vec{P}(\vec{R},t)}{\varepsilon(\infty)} \quad\Rightarrow\quad \hat{q}.\vec{E}(\vec{q}) = -\frac{\vec{P}(\vec{q}).\hat{q}}{\varepsilon(\infty)}$$

The above two imply that the E-field has non-zero component only in the direction parallel to $\vec{q}$ given by:

$$\vec{E}(\vec{q}) = -\frac{\vec{P}(\vec{q}).\hat{q}}{\varepsilon(\infty)}\hat{q}$$

Optical Phonons in Polar Crystals: TO Phonons

Subtract the two equations and take the limit $q \approx 0$ to get:

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})] = -\frac{\alpha}{M_r}\sum_j \left[\left[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})\right].\hat{n}_j\right]\hat{n}_j + \frac{f}{M_r}\vec{E}(\vec{q})$$

Transverse Optical Phonons:

Take the cross-product of both sides with $\hat{q}$ to get:

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})]\times\hat{q} = -\frac{\alpha}{M_r}\sum_j \left[\left[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})\right].\hat{n}_j\right]\hat{n}_j\times\hat{q} + \frac{f}{M_r}\vec{E}(\vec{q})\times\hat{q}$$

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})]\times\hat{q} = -\frac{b\alpha}{M_r}[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})]\times\hat{q}$$

$$\sum_j \hat{n}_j\,\hat{n}_j = b \qquad \sum_j\left(\vec{A}.\hat{n}_j\right)\left(\hat{n}_j\times\hat{q}\right) = b\vec{A}\times\hat{q}$$

$$\Rightarrow \omega = \sqrt{\frac{b\alpha}{M_r}}$$

$$\Rightarrow \omega_{TO}(q\approx 0) = \sqrt{\frac{b\alpha}{M_r}}$$

For example in GaAs:

$$\vec{n}_1 = \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix} \quad \vec{n}_2 = \frac{1}{\sqrt{3}}\begin{bmatrix}-1\\-1\\1\end{bmatrix} \quad \vec{n}_3 = \frac{1}{\sqrt{3}}\begin{bmatrix}-1\\1\\-1\end{bmatrix} \quad \vec{n}_4 = \frac{1}{\sqrt{3}}\begin{bmatrix}1\\-1\\-1\end{bmatrix}$$

$$\Rightarrow \sum_j \hat{n}_j\,\hat{n}_j = \frac{4}{3}\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix} = \frac{4}{3}$$

Optical Phonons in Polar Crystals: LO Phonons

Again start from:

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})] = -\frac{\alpha}{M_r}\sum_j \left[\left[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})\right].\hat{n}_j\right]\hat{n}_j + \frac{f}{M_r}\vec{E}(\vec{q})$$

Longitudinal Optical Phonons:

Take the dot-product of both sides with $\hat{q}$ to get:

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})].\hat{q} = -\frac{\alpha}{M_r}\sum_j \left[\left[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})\right].\hat{n}_j\right]\hat{n}_j.\hat{q} + \frac{f}{M_r}\vec{E}(\vec{q}).\hat{q}$$

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})].\hat{q} = -\frac{b\alpha}{M_r}[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})].\hat{q} - \frac{nf^2}{M_r\varepsilon(\infty)}[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})].\hat{q}$$

$$\sum_j \hat{n}_j\,\hat{n}_j = b \qquad \sum_j\left(\vec{A}.\hat{n}_j\right)\left(\hat{n}_j.\hat{q}\right) = b\vec{A}.\hat{q}$$

$$\Rightarrow \omega_{LO}(q\approx 0) = \sqrt{\frac{b\alpha}{M_r} + \frac{nf^2}{M_r\varepsilon(\infty)}}$$

$$\Rightarrow \omega_{LO}^2(q\approx 0) - \omega_{TO}^2(q\approx 0) = \frac{nf^2}{M_r\varepsilon(\infty)}$$

$$\Rightarrow \omega_{LO}^2 - \omega_{TO}^2 = \frac{nf^2}{M_r\varepsilon(\infty)}$$

Optical Phonons in Polar Crystals: Dielectric Constant

Consider the response of polar optical phonons to an externally applied E-field
The total electric field (external plus internal) is:

$$\vec{E}(\vec{R},t) = \vec{E}(\vec{q})\, e^{i\vec{q}.\vec{R}-i\omega t} \qquad \left\{ \; \vec{q} \approx 0 \right.$$

We have:

$$-\omega^2[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})] = -\frac{\alpha}{M_r}\sum_j [[\,\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})].\hat{n}_j]\hat{n}_j + \frac{f}{M_r}\vec{E}(\vec{q})$$

$$\Rightarrow [\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})] = -\frac{\frac{f}{M_r}\vec{E}(\vec{q})}{\omega^2-\omega_{TO}^2} \qquad \left\{ \sum_j \hat{n}_j\,\hat{n}_j = b \right.$$

$$\Rightarrow \vec{P}(\vec{q}) = nf[\vec{u}_2(\vec{q})-\vec{u}_1(\vec{q})] = -\frac{\frac{nf^2}{M_r}\vec{E}(\vec{q})}{\omega^2-\omega_{TO}^2}$$

The D-field is:

$$\vec{D}(\vec{q}) = \varepsilon(\infty)\vec{E}(\vec{q}) + \vec{P}(\vec{q}) = \varepsilon(\omega)\vec{E}(\vec{q})$$

$$\Rightarrow D(\vec{q}) = \left(\varepsilon(\infty) - \frac{nf^2/M_r}{\omega^2-\omega_{TO}^2}\right)\vec{E}(\vec{q})$$

$$\Rightarrow \varepsilon(\omega) = \varepsilon(\infty) - \frac{nf^2/M_r}{\omega^2-\omega_{TO}^2}$$

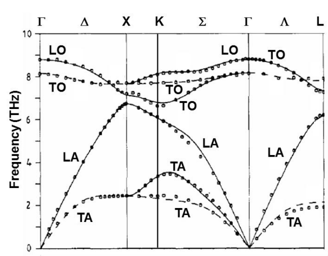
Optical Phonons in Polar Crystals: Lydanne-Sachs-Teller Relation

We have:

$$\varepsilon(\omega) = \varepsilon(\infty) - \frac{nf^2/M_r}{\omega^2-\omega_{TO}^2}$$

$$\Rightarrow \varepsilon(0) = \varepsilon(\infty) + \frac{nf^2/M_r}{\omega_{TO}^2} \longrightarrow \text{Low frequency dielectric constant}$$

$$\Rightarrow \frac{nf^2}{M_r} = \omega_{TO}^2[\varepsilon(0)-\varepsilon(\infty)]$$



The LO-TO phonon frequency splitting was given by:

$$\Rightarrow \omega_{LO}^2 - \omega_{TO}^2 = \frac{nf^2}{M_r\varepsilon(\infty)} = \omega_{TO}^2\frac{[\varepsilon(0)-\varepsilon(\infty)]}{\varepsilon(\infty)}$$

$$\Rightarrow \omega_{LO}^2 = \omega_{TO}^2\frac{\varepsilon(0)}{\varepsilon(\infty)}$$

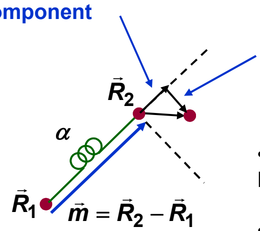
The above relationship is called the Lydanne-Sachs-Teller relation
The above relation does not change if more than nearest-neighbor interactions are also included in the analysis
One can also write:

$$\varepsilon(\omega) = \varepsilon(\infty) - \frac{\omega_{TO}^2[\varepsilon(0)-\varepsilon(\infty)]}{\omega^2-\omega_{TO}^2}$$

Vector Dynamical Equations: Bond-Stretching and Bond-Bending

Bond-stretching component

Bond-bending component



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

$\hat{m} = \dfrac{\vec{m}}{|\vec{m}|}$

- In general, atomic displacements can cause both bond-stretching and bond-bending
- Both bond-stretching and bond-bending give rise to restoring forces

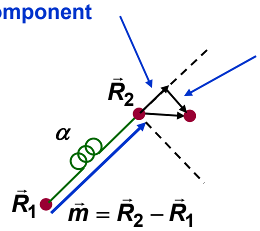
Bond-stretching contribution:

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

Vector Dynamical Equations: Bond-Stretching and Bond-Bending

Bond-stretching component

Bond-bending component



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

$\hat{m} = \dfrac{\vec{m}}{|\vec{m}|}$

First find two mutually orthogonal unit vectors that are also perpendicular to $\hat{m}$

Let these be: $\hat{n}_1$ and $\hat{n}_2$

Bond-stretching and bond-bending contributions:

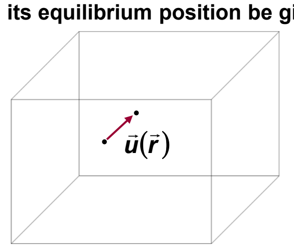
$$\begin{aligned} M\,\frac{d^2\vec{u}(\vec{R}_1,t)}{dt^2} = {} & \alpha\left[\left[\vec{u}(\vec{R}_1+\vec{m},t)-\vec{u}(\vec{R}_1,t)\right].\,\hat{m}\right]\hat{m} \\ & +\beta\left[\left[\vec{u}(\vec{R}_1+\vec{m},t)-\vec{u}(\vec{R}_1,t)\right].\,\hat{n}_1\right]\hat{n}_1 \\ & +\beta\left[\left[\vec{u}(\vec{R}_1+\vec{m},t)-\vec{u}(\vec{R}_1,t)\right].\,\hat{n}_2\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

Macroscopic Description of Acoustic Phonons in Solids

Acoustic phonons can also be described using a macroscopic formalism based on the theory of elasticity

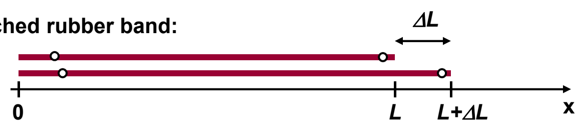
Let the local displacement of a solid from its equilibrium position be given by the vector

$$\vec{u}(\vec{r}) = \begin{bmatrix} u_x(\vec{r}) \\ u_y(\vec{r}) \\ u_z(\vec{r}) \end{bmatrix}$$



Strain Tensor:

Consider a stretched rubber band:



There is a uniform strain given by:

$$e_{xx} = \frac{\partial u_x(x)}{\partial x} = \frac{\Delta L}{L}$$

Stress and Strain

Strain Tensor:

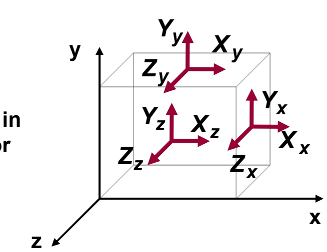
The strain tensor $\overline{\overline{e}}$ is defined by its 6 components:

$$e_{xx} = \frac{\partial u_x(\vec{r})}{\partial x} \quad e_{yy} = \frac{\partial u_y(\vec{r})}{\partial y} \quad e_{zz} = \frac{\partial u_z(\vec{r})}{\partial z}$$

$$e_{xy} = \frac{\partial u_x(\vec{r})}{\partial y} + \frac{\partial u_y(\vec{r})}{\partial x} \quad e_{yz} = \frac{\partial u_y(\vec{r})}{\partial z} + \frac{\partial u_z(\vec{r})}{\partial y} \quad e_{zx} = \frac{\partial u_z(\vec{r})}{\partial x} + \frac{\partial u_x(\vec{r})}{\partial z}$$

Stress Tensor:

Stress is the force acting per unit area on any plane of the solid
It is a tensor with 9 components (as shown)



For example, X_y is the force acting per unit area in the x-direction on a plane that has a normal vector pointing in the y-direction

Hooke's Law

Stress Tensor:

In solids with cubic symmetry, if the stress tensor produces no torque (and no angular acceleration) then one must have:

$$X_y = Y_x \qquad Y_z = Z_y \qquad Z_x = X_z$$

So there are only 6 independent stress tensor components:

$$X_x \quad Y_y \quad Z_z \quad Y_z \quad Z_x \quad X_y$$

Hooke's Law:

A fundamental theorem in the theory of elasticity is Hooke's law that says that strain is proportional to the stress and vice versa. Mathematically, the 6 stress tensor components are related to the 6 strain tensor components by a matrix:

$$\begin{bmatrix} X_x \\ Y_y \\ Z_z \\ Y_z \\ Z_x \\ X_y \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & . & . & c_{16} \\ c_{21} & c_{22} & . & . & . & . \\ c_{31} & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ c_{61} & c_{62} & . & . & . & c_{66} \end{bmatrix} \begin{bmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{bmatrix}$$

Elastic stiffness constants

Hooke's Law for Cubic Materials

In solids with cubic symmetry (SC, FCC, BCC) the matrix of elastic constants have only three independent components:

$$\begin{bmatrix} X_x \\ Y_y \\ Z_z \\ Y_z \\ Z_x \\ X_y \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} \begin{bmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{bmatrix}$$

Elastic energy:

The elastic energy per unit volume of a strained cubic material is:

$$V = \frac{1}{2}c_{11}\left(e_{xx}^2 + e_{yy}^2 + e_{zz}^2\right) + c_{12}\left(e_{xx}e_{yy} + e_{yy}e_{zz} + e_{zz}e_{xx}\right) + c_{44}\left(e_{yz}^2 + e_{zx}^2 + e_{xy}^2\right)$$

Wave Equation for Acoustic Phonons in Cubic Solids

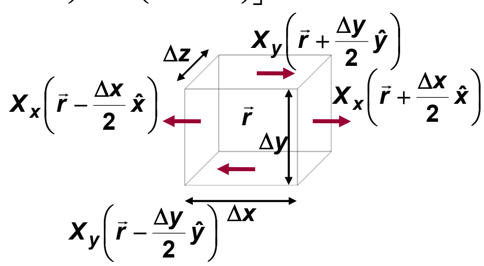
Consider a solid with density ρ

Consider a small volume of this solid that is in motion, as shown

We want to write Newton's second law for its motion in the x-direction
First consider only the force due to the stress tensor component X_x

$$\rho\,\Delta x\,\Delta y\,\Delta z\,\frac{\partial^2 u_x(\vec{r},t)}{\partial t^2}=\Delta y\,\Delta z\left[X_x\left(\vec{r}+\frac{\Delta x}{2}\hat{x}\right)-X_x\left(\vec{r}-\frac{\Delta x}{2}\hat{x}\right)\right]=\Delta x\,\Delta y\,\Delta z\,\frac{\partial X_x(\vec{r})}{\partial x}$$

$$\Rightarrow \rho\,\frac{\partial^2 u_x(\vec{r},t)}{\partial t^2}=\frac{\partial X_x(\vec{r})}{\partial x}$$



Now add the contribution of all forces acting in the x-direction:

$$\rho\,\frac{\partial^2 u_x(\vec{r},t)}{\partial t^2}=\frac{\partial X_x(\vec{r})}{\partial x}+\frac{\partial X_y(\vec{r})}{\partial y}+\frac{\partial X_z(\vec{r})}{\partial z}$$

Wave Equation for Acoustic Phonons in Cubic Solids

We have:

$$\rho\,\frac{\partial^2 u_x(\vec{r},t)}{\partial t^2}=\frac{\partial X_x(\vec{r})}{\partial x}+\frac{\partial X_y(\vec{r})}{\partial y}+\frac{\partial X_z(\vec{r})}{\partial z}$$

Similarly for acceleration in the y- and z-directions we get:

$$\rho\,\frac{\partial^2 u_y(\vec{r},t)}{\partial t^2}=\frac{\partial Y_x(\vec{r})}{\partial x}+\frac{\partial Y_y(\vec{r})}{\partial y}+\frac{\partial Y_z(\vec{r})}{\partial z}\qquad \rho\,\frac{\partial^2 u_z(\vec{r},t)}{\partial t^2}=\frac{\partial Z_x(\vec{r})}{\partial x}+\frac{\partial Z_y(\vec{r})}{\partial y}+\frac{\partial Z_z(\vec{r})}{\partial z}$$

Using the Hooke's law relation, the above equation for motion in the x-direction can be written as:

$$\rho\,\frac{\partial^2 u_x(\vec{r},t)}{\partial t^2}=c_{11}\frac{\partial e_{xx}(\vec{r})}{\partial x}+c_{12}\left[\frac{\partial e_{yy}(\vec{r})}{\partial x}+\frac{\partial e_{zz}(\vec{r})}{\partial x}\right]+c_{44}\left[\frac{\partial e_{xy}(\vec{r})}{\partial y}+\frac{\partial e_{zx}(\vec{r})}{\partial z}\right]$$

$$=c_{11}\frac{\partial^2 u_x(\vec{r})}{\partial x^2}+c_{44}\left[\frac{\partial^2 u_x(\vec{r})}{\partial y^2}+\frac{\partial^2 u_x(\vec{r})}{\partial z^2}\right]+(c_{12}+c_{44})\left[\frac{\partial^2 u_y(\vec{r})}{\partial x\,\partial y}+\frac{\partial^2 u_z(\vec{r})}{\partial x\,\partial z}\right]$$

Wave equation for acoustic phonons

Wave Equation for Acoustic Phonons in Cubic Solids

$$\rho \frac{\partial^2 u_x(\vec{r},t)}{\partial t^2} = c_{11}\frac{\partial^2 u_x(\vec{r})}{\partial x^2} + c_{44}\left[\frac{\partial^2 u_x(\vec{r})}{\partial y^2} + \frac{\partial^2 u_x(\vec{r})}{\partial z^2}\right] + (c_{12}+c_{44})\left[\frac{\partial^2 u_y(\vec{r})}{\partial x\,\partial y} + \frac{\partial^2 u_z(\vec{r})}{\partial x\,\partial z}\right]$$

LA phonons:

Consider a LA phonon wave propagating in the x-direction:

$$u_x(\vec{r},t) = A\, e^{i\,q_x x} e^{-i\,\omega\, t}$$

Plug the assumed solution in the wave equation to get:

$$\omega = \sqrt{\frac{c_{11}}{\rho}}\, q_x \longrightarrow \text{velocity of wave} = \sqrt{\frac{c_{11}}{\rho}}$$

TA phonons:

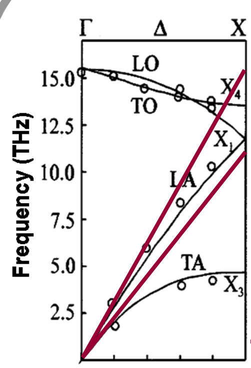
Consider a TA phonon wave propagating in the y-direction:

$$u_x(\vec{r},t) = A\, e^{i\,q_y y} e^{-i\,\omega\, t}$$

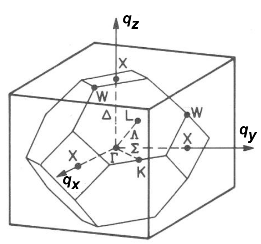
Plug the assumed solution in the wave equation to get:

$$\omega = \sqrt{\frac{c_{44}}{\rho}}\, q_y \longrightarrow \text{velocity of wave} = \sqrt{\frac{c_{44}}{\rho}}$$

Acoustic Phonons in Silicon



Results from elasticity theory



In Silicon:

$$c_{11} = 1.66\times10^{11} \quad \text{N/m}^2$$
$$c_{12} = 0.64\times10^{11} \quad \text{N/m}^2$$
$$c_{44} = 0.80\times10^{11} \quad \text{N/m}^2$$
$$\rho = 2330 \quad \text{kg/m}^3$$

For LA phonons propagating in the Γ-X direction:

$$\text{velocity of wave} = \sqrt{\frac{c_{11}}{\rho}} = 8.44 \ \text{km/sec}$$

For TA phonons propagating in the Γ-X direction:

$$\text{velocity of wave} = \sqrt{\frac{c_{44}}{\rho}} = 5.86 \ \text{km/sec}$$

Wave Equation for Acoustic Phonons in Cubic Solids

$$\rho\frac{\partial^2 u_x(\vec{r},t)}{\partial t^2} = c_{11}\frac{\partial^2 u_x(\vec{r})}{\partial x^2} + c_{44}\left[\frac{\partial^2 u_x(\vec{r})}{\partial y^2} + \frac{\partial^2 u_x(\vec{r})}{\partial z^2}\right] + (c_{12}+c_{44})\left[\frac{\partial^2 u_y(\vec{r})}{\partial x\,\partial y} + \frac{\partial^2 u_z(\vec{r})}{\partial x\,\partial z}\right]$$

$$\rho\frac{\partial^2 u_y(\vec{r},t)}{\partial t^2} = c_{11}\frac{\partial^2 u_y(\vec{r})}{\partial y^2} + c_{44}\left[\frac{\partial^2 u_y(\vec{r})}{\partial z^2} + \frac{\partial^2 u_y(\vec{r})}{\partial x^2}\right] + (c_{12}+c_{44})\left[\frac{\partial^2 u_x(\vec{r})}{\partial x\,\partial y} + \frac{\partial^2 u_z(\vec{r})}{\partial z\,\partial y}\right]$$

Consider a phonon wave propagating in the direction: $\frac{\hat{x}+\hat{y}}{\sqrt{2}} \quad \Rightarrow \quad \vec{q} = q\frac{\hat{x}+\hat{y}}{\sqrt{2}}$

$$\begin{bmatrix} u_x(\vec{r},t) \\ u_y(\vec{r},t) \end{bmatrix} = \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} e^{i\,\vec{q}\,.\,\vec{r}}\,e^{-i\,\omega\,t}$$

Plug the assumed solution in the wave equation to get two coupled equations:

$$\begin{bmatrix} \frac{q^2}{2}(c_{11}+c_{44}) & \frac{q^2}{2}(c_{12}+c_{44}) \\ \frac{q^2}{2}(c_{12}+c_{44}) & \frac{q^2}{2}(c_{11}+c_{44}) \end{bmatrix} \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = \rho\,\omega^2 \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix}$$

Wave Equation for Acoustic Phonons in Cubic Solids

$$\begin{bmatrix} \frac{q^2}{2}(c_{11}+c_{44}) & \frac{q^2}{2}(c_{12}+c_{44}) \\ \frac{q^2}{2}(c_{12}+c_{44}) & \frac{q^2}{2}(c_{11}+c_{44}) \end{bmatrix} \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = \rho\,\omega^2 \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix}$$

The two solutions are as follows:

LA phonon:

$$\omega = \sqrt{\frac{c_{11}+c_{12}+2c_{44}}{2\rho}}\,q \qquad \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = A\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

TA phonon:

$$\omega = \sqrt{\frac{c_{11}-c_{12}}{2\rho}}\,q \qquad \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = A\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$