

Theory of Semiconductor Devices (반도체 소자 이론)

Lecture 12

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Lattice Vibration

- In a *perfect periodic structure* the atoms are *assumed to be fixed* at the basis sites of a Bravais lattice. We know, however, that the atoms exhibit *random thermal vibrations* around their equilibrium positions, where the *amplitude of the vibrations depends on temperature*.
- Because of the bonding forces that produce the crystal structure, the random motion of *individual atoms are strongly coupled* to one another. This coupling produces *random wave propagation* in the crystal.
- When electrons and holes move through this crystal of randomly vibrating atoms, they can *exchange energy and momentum* with the atoms.
- In this manner the *charge carriers are scattered by the thermal vibrations of the crystal* and a thermodynamic equilibrium is established between the crystal and the electrons and holes.
- Since these scattering events play an important role in the transport properties of semiconductors, it is necessary to obtain a mathematical description of lattice vibrations.

Lattice Vibration - Example

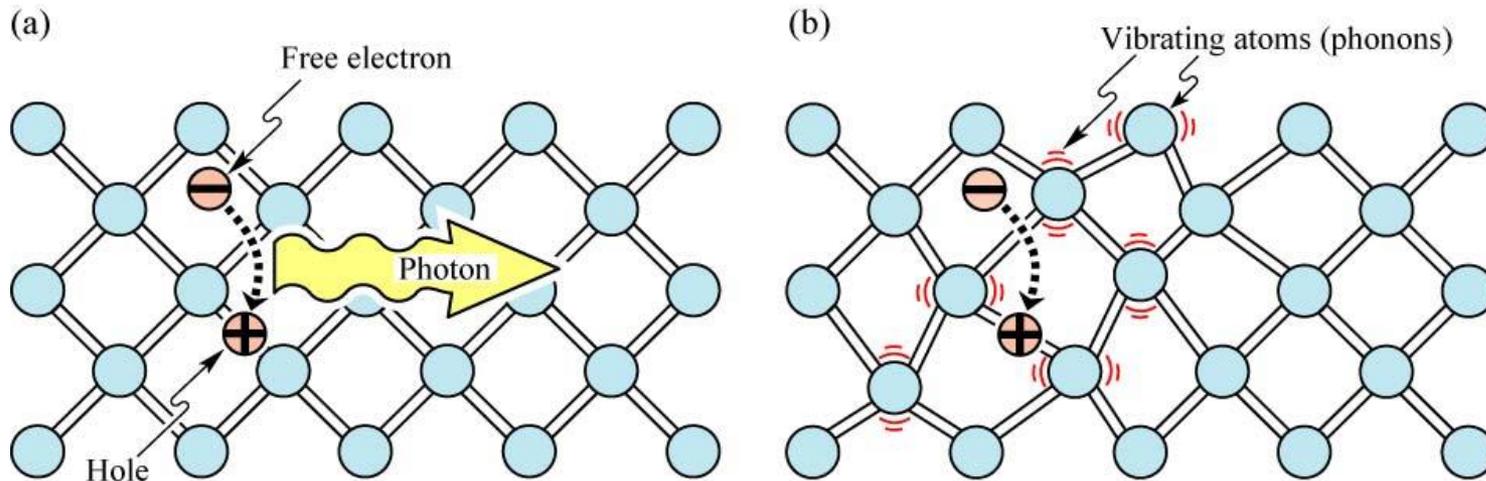


Fig. 2.5. (a) Radiative recombination of an electron-hole pair accompanied by the emission of a photon with energy $h\nu \approx E_g$. (b) In non-radiative recombination events, the energy released during the electron-hole recombination is converted to phonons (adopted from Shockley, 1950).

E. F. Schubert
Light-Emitting Diodes (Cambridge Univ. Press)
www.LightEmittingDiodes.org

Lattice Vibration

- Let us first define a vector $\mathbf{u}_{R,d}$ which indicates the **displacement of an atom from its equilibrium position** given by **basis vector \mathbf{d}** and **direct lattice vector \mathbf{R}** . We take \mathbf{R} to represent a particular primitive unit cell and \mathbf{d} to represent the position of each atom in the unit cell.
- Thus, \mathbf{R} and \mathbf{d} index every atom in the crystal.
- The mass of each atom is M_d so that \mathbf{d} indexes atoms of different mass in each primitive unit cell. Using these definitions the kinetic energy of all the atoms in the crystal is

$$T = \sum_{R,d} \frac{1}{2} M_d |\dot{\mathbf{u}}_{R,d}|^2 \quad (3.64)$$

where $\dot{\mathbf{u}}_{R,d}$ indicates the total derivative with respect to time. In (3.64) the sum in \mathbf{R} is taken over the N unit cells and the sum in \mathbf{d} is taken over the n atoms per unit cell.

- We next assume that the potential energy of the atoms in the crystal, U depends on the displacements, $\mathbf{u}_{R,d}$, and has a minimum, U_0 when all atoms are in their equilibrium positions $\mathbf{u}_{R,d} = 0$. If we resolve $\mathbf{u}_{R,d}$ into Cartesian components,

$$\mathbf{u}_{R,d} = \sum_j u_{j,R,d} \hat{j}, \quad \hat{j} = \hat{x}, \hat{y}, \hat{z} \quad (3.65)$$

Lattice Vibration

we can expand the potential energy in a power series **around the minimum potential energy** as

$$\begin{aligned}
 U = U_0 + \sum_{j,R,d} \left[\frac{\partial U}{\partial u_{j,R,d}} \right]_0 u_{j,R,d} \\
 + \frac{1}{2} \sum_{j,R,d,j',R',d'} \left[\frac{\partial^2 U}{\partial u_{j,R,d} \partial u_{j',R',d'}} \right]_0 u_{j,R,d} u_{j',R',d'} + \dots \quad (3.66)
 \end{aligned}$$

Since the expansion is **around the minimum potential energy point**, the slope $[\partial U / \partial u_{j,R,d}]_0$ is **zero**. For **small displacements**, we can neglect higher-order terms and approximate the potential energy as

$$U = U_0 + \frac{1}{2} \sum_{j,R,d,j',R',d'} \left[\frac{\partial^2 U}{\partial u_{j,R,d} \partial u_{j',R',d'}} \right]_0 u_{j,R,d} u_{j',R',d'} \quad (3.67)$$

We can obtain the classical equations of motion for the atoms of the crystal with **Lagrange's formulation**

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{u}} \right) - \frac{\partial L}{\partial u} = 0 \quad (3.68)$$

where

$$L = T - U \quad (3.69)$$

Lattice Vibration

Using (3.64) and (3.67) in (3.69) and (3.68), we have

$$M_d \ddot{u}_{j,R,d} = - \frac{1}{2} \sum_{j',R',d'} \left[\frac{\partial^2 U}{\partial u_{j,R,d} \partial u_{j',R',d'}} \right]_0 u_{j',R',d'} \quad (3.70)$$

Equation (3.70) can be simplified somewhat by writing it in vector notation as

$$M_d \ddot{\mathbf{u}}_{R,d} = \frac{1}{2} \sum_{R',d'} [\mathbf{A}_{R,d,R',d'}] \cdot \mathbf{u}_{R',d'} \quad (3.71)$$

where $[\mathbf{A}_{R,d,R',d'}]$ is a coupling tensor consisting of the terms $[\partial^2 U / \partial u_{j,R,d} \partial u_{j',R',d'}]_0$.

- Notice that (3.71) has the **form of Newton's law**, Each term on the right-hand side of (3.71) represents the force exerted on **d** atom in **R** unit cell through the coupling tensor by a displacement of **d'** atom in **R'** unit cell.
- We also see that (3.71) represents a large number of **coupled differential equations** in very compact form. There are three Cartesian equations for each of n atoms in N unit cells, for a total of $3nN$ equations.
- We know intuitively, however, that the force terms on the right-hand side of (3.71) cannot depend on the absolute position of the atoms but only on the **relative spacing** between them.

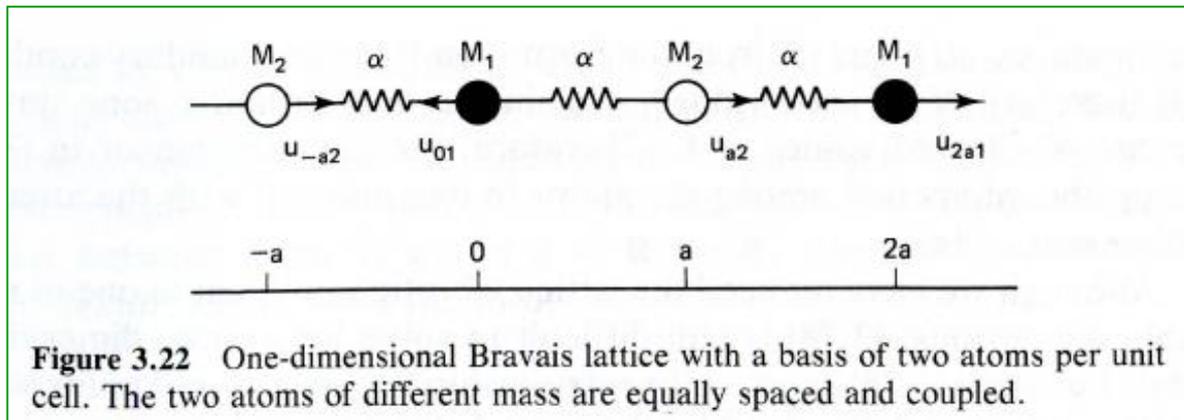
Lattice Vibration

--- Skip from (3.72) to (3.78) ---

- To understand some of the basic features of vibrational frequency bands, let us examine a *one-dimensional Bravais lattice with a basis of two atoms per unit cell*.
- As shown in Fig. 3.22, we assume that the atoms have masses M_1 and M_2 , are equally spaced at a distance a , and have a *coupling coefficient* α .
- We will consider interactions between nearest neighbors only. From (3.72) the equations of motion are

$$M_1 \ddot{u}_{01} = -\frac{1}{2} \alpha [(u_{01} - u_{a2}) + (u_{01} - u_{-a2})] \quad (3.79)$$

$$M_2 \ddot{u}_{a2} = -\frac{1}{2} \alpha [(u_{a2} - u_{2a1}) + (u_{a2} - u_{01})]$$



Lattice Vibration

- Expressions for the displacement of each atom are given by (3.73) as

$$\begin{aligned}
 u_{01} &= u_1 \exp[-i\omega_s t] \\
 u_{a2} &= u_2 \exp[i(q_s a - \omega_s t)] \\
 u_{2a1} &= u_1 \exp[i(2q_s a - \omega_s t)] \\
 u_{-a2} &= u_2 \exp[i(-q_s a - \omega_s t)]
 \end{aligned}
 \tag{3.80}$$

Using (3.80) in (3.79), we have

$$\begin{aligned}
 \omega_s^2 M_1 u_1 &= \alpha(u_1 - u_2 \cos q_s a) \\
 \omega_s^2 M_2 u_2 &= \alpha(u_2 - u_1 \cos q_s a)
 \end{aligned}
 \tag{3.81}$$

The coupled set of equations (3.81) can be put in matrix form as

$$\begin{bmatrix} \alpha - \omega_s^2 M_1 & -\alpha \cos q_s a \\ -\alpha \cos q_s a & \alpha - \omega_s^2 M_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = 0
 \tag{3.82}$$

Lattice Vibration

- Equation (3.82) is similar to (2.63) for the nearly free electron energy bands .
- To keep the displacements from vanishing identically, the determinant of coefficients for the matrix must be set equal to zero. Solving for the frequency, we obtain

$$\omega_{s\pm}^2 = \frac{\alpha}{2} \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm \frac{\alpha}{2} \left[\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 q_s a}{M_1 M_2} \right]^{1/2} \quad (3.83)$$

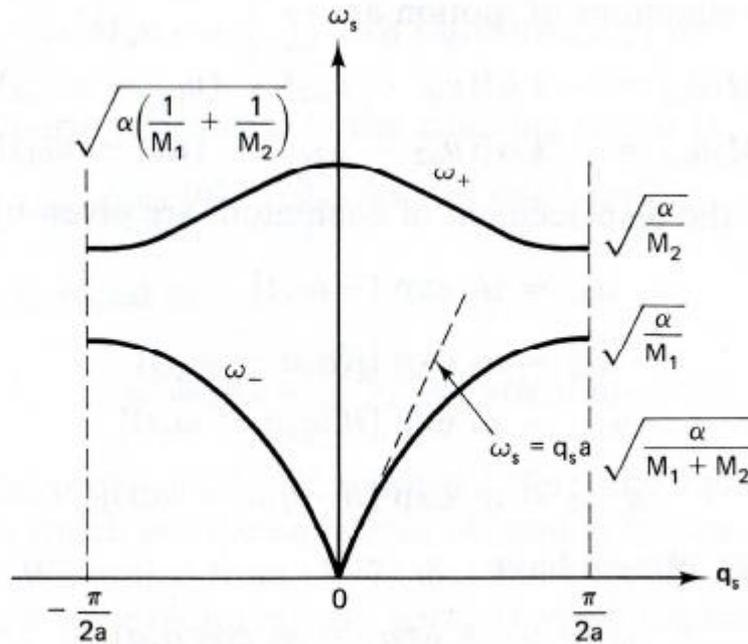


Figure 3.23 Vibrational frequency bands for a one-dimensional Bravais lattice with a basis of two atoms in the first Brillouin zone.

- Equation (3.83) tells us that the vibrational frequency spectrum has **two allowed bands separated by a forbidden gap**. The results are plotted versus wavevector in Fig. 3.23.

Lattice Vibration

- For small values of \mathbf{q}_s , the low-frequency band, ω_{s-} , is linearly dependent on \mathbf{q}_s . Since this relationship between frequency and wavevector is a characteristic of elastic waves in continuous media, ω_{s-} is referred to as an **acoustic band**. As a result of this dependence, the group velocity $d\omega_s/dq_s$ and the phase velocity ω_s/q_s are approximately given by the velocity of **sound** in the material. Also, for this band the two atoms in each unit cell have displacements that are about **in phase**.

- For the much higher frequency band, ω_{s+} , near $\mathbf{q}_s = 0$, however, the two atoms in each unit cell have displacements that are in **opposite directions** at any instant of time.

- This motion produces the **maximum relative displacement** between atoms, which, from (3.72), gives the **maximum restoring force** and thus the **highest vibrational frequency**.

- In ionic crystals this opposing motion of positively and negatively charged atoms in a unit cell results in an oscillating dipole moment which interacts strongly with electromagnetic radiation.

- For this reason ω_{s+} is called an **optical band**.

<http://physics.ucsc.edu/~bridges/simulations/index.html>

https://www.youtube.com/watch?v=M4WQs_U1nmU

Lattice Vibration

- We have seen that the random thermal motion of the atoms in a crystal can be described by displacement vectors, $\mathbf{u}_{R,d}(t)$, given by (3.73).
- From the classical equations of motion, we were able to deduce the relationship between the frequency and wavevector of these displacement vectors.
- To determine the **energy of the lattice vibrations**, a Hamiltonian for the crystal can be constructed from the **kinetic energy terms** of (3.64) and the **potential energy terms** of (3.67).
- The result constitutes the Hamiltonian for a set of **harmonic oscillators**. This Hamiltonian can then be used in Schrodinger's equation to determine the energy of the system. However, the solution for a **quantum harmonic oscillator** is well known.
- We can use this result to obtain the total lattice energy as the sum of energies from each vibrational mode,

$$\mathcal{E} = U_0 + \sum_{j,d,q_s} \mathcal{E}_{j,d,q_s} \quad (3.84)$$

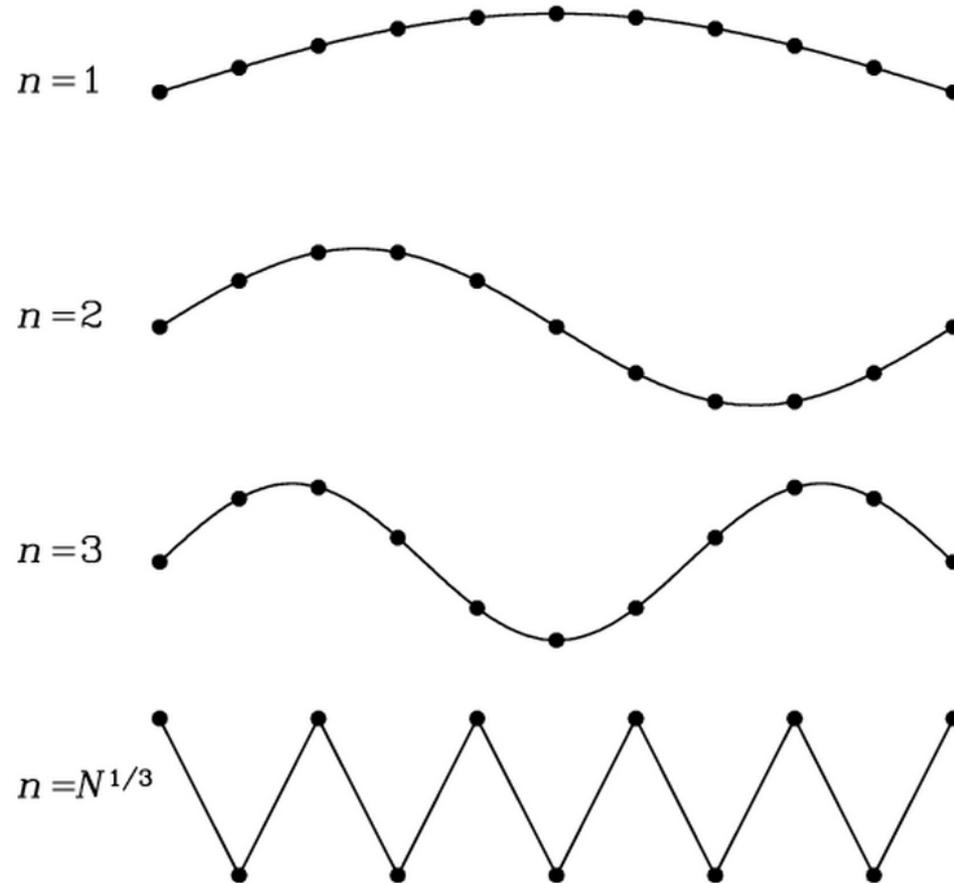
where

$$\mathcal{E}_{j,d,q_s} = \hbar\omega_{j,d}(n_{q_s} + \frac{1}{2}), \quad n_{q_s} = 0, 1, 2, \dots \quad (3.85)$$

In (3.84) the summation in \mathbf{q}_s is over all N vibrational modes in the first Brillouin zone, in \mathbf{d} over the one acoustic and $(n - 1)$ optical bands, and in j over the one longitudinal and two transverse bands.

Lattice Vibration - Modes

Lattice Vibration Modes

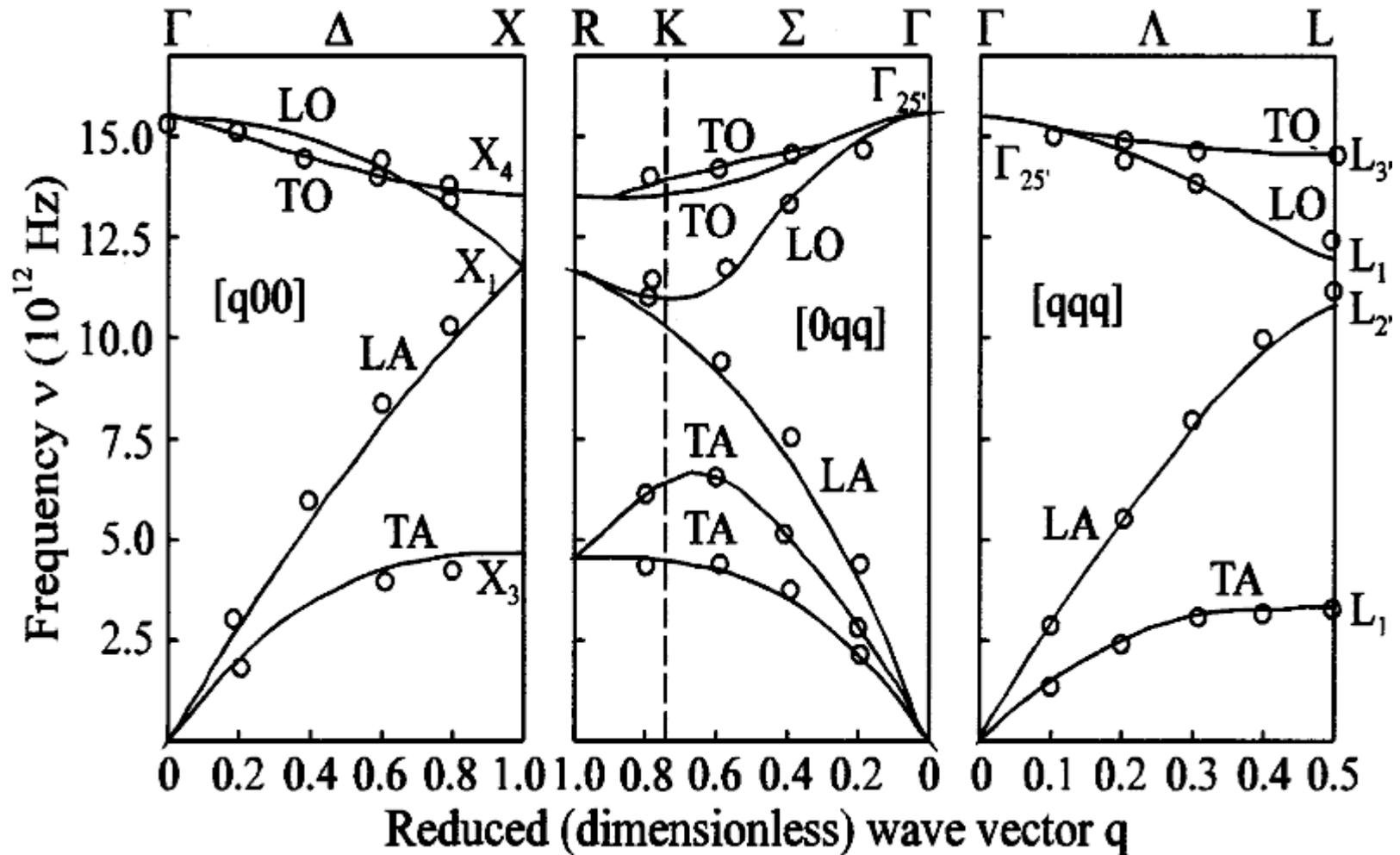


Lattice Vibration

- For (3.85) n_{q_s} is the excitation state of a lattice vibrational mode indexed by \mathbf{q}_s . Since n_{q_s} can take on only *integer* values, we see that each vibrational mode \mathbf{q}_s can only **gain** or **lose energy in quanta** of $\hbar\omega_s$. This behavior is **exactly analogous to the quanta of electromagnetic radiation in a cavity**.
- Electromagnetic quanta are referred to as *photons*.
- For this reason **lattice vibrational quanta are called phonons**. The excitation state of a given mode, n_{q_s} , is then taken as the number of phonons in that mode.
- The advantage of using the **phonon-particle concept** rather than the **vibrational mode-wave concept** is that a **phonon interacts with other particles as if it had momentum $\hbar\mathbf{q}_s$ and energy $\hbar\omega_{j,d}$** .
- Phonons are *classified* according to their **frequency band**. That is, depending on whether j is **transverse** (T) or **longitudinal** (L) and \mathbf{d} is **acoustic** (A) or **optical** (O), a phonon is a **transverse acoustic** (TA), a **transverse optical** (TO), a **longitudinal acoustic** (LA), or a **longitudinal optical** (LO) phonon.

<https://www.youtube.com/watch?v=jAXx0018QCc&nohtml5=False>

Lattice Vibration - Si



Lattice Vibration

Longitudinal and transverse optical phonon frequencies near $\mathbf{q}_s = 0$ are listed in Table 3.2 for a number of semiconductors.

TABLE 3.2 Longitudinal and Transverse Optical Phonon Frequencies in 10^{12} Hz

	ω_{LO}	ω_{TO}		ω_{LO}	ω_{TO}
C	39.96	39.96	InP	10.35	9.10
SiC	29.15	23.90	InAs	7.30	6.57
Si	15.69	15.69	InSb	6.00	5.37
Ge	9.02	9.02	ZnO	17.4	11.8
BN	40.20	31.95	ZnS	10.47	8.22
BP	25.0	24.6	ZnSe	7.53	6.12
AlN	27.5	20.0	ZnTe	6.18	5.47
AlP	15.03	13.20	CdS	9.1	6.9
AlSb	10.20	9.60	CdSe	6.52	5.13
GaN	24.0	16.5	CdTe	5.13	4.20
GaP	12.08	10.96			
GaAs	8.76	8.06			
GaSb	7.30	6.90			