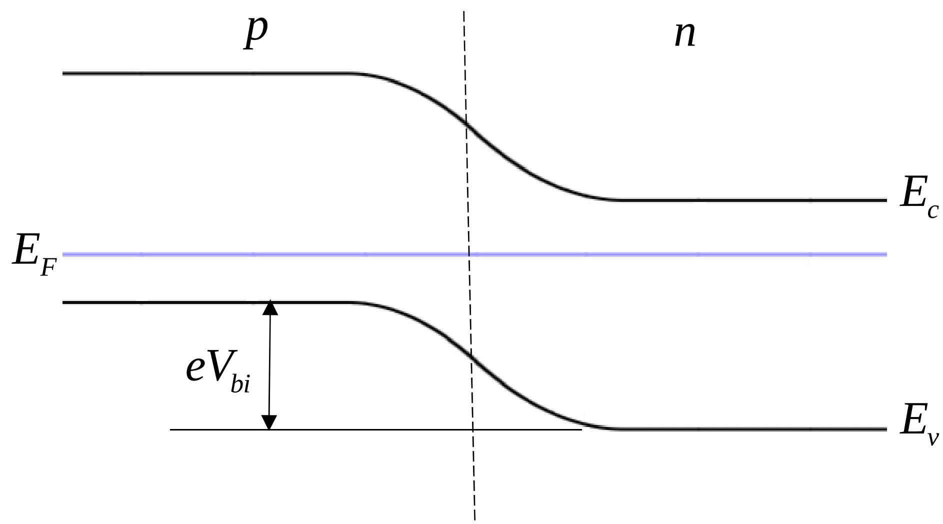
Technische Universität Graz

9. Semiconductor Devices /Phonons

Oct 29, 2018

p and n profiles



$V_{bi} \sim 1$ V

$W \sim 1$ μm

$E_{max} \sim 10^4$ V/cm

$$p = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right) \qquad n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

The electric field pushes the electrons towards the n-region and the holes towards the p-region.

Diffusion sends electrons towards the p-region and holes towards the n-region.

Abrupt pn junctions in the depletion approximation

In an abrupt pn junction, the doping changes abruptly from p to n. It is common to solve for the band bending, the local electric field, the carrier concentration profiles, and the local conductivity in the depletion approximation. In this approximation it is assumed that there is a depletion width W around the transition from p to n where the charge carrier densities are negligible. Outside the depletion width the charge carrier densities are equal to the doping densities so that the semiconductor is electrically neutral outside the depletion width. Using this approximation it is possible to calculate the important properties of the pn junction.

N_A = 1E15 1/cm³ N_D = 1E15 1/cm³ E_g = 1.166-4.73E-4*T*T/(T+636) eV

$N_v(300)$ = 9.84E18 1/cm³ $N_c(300)$ = 2.78E19 1/cm³ ϵ_r = 12 T = 300 K

μ_p = 480 cm²/V s μ_n = 1350 cm²/V s τ_p = 1E-10 s τ_n = 1E-10 s

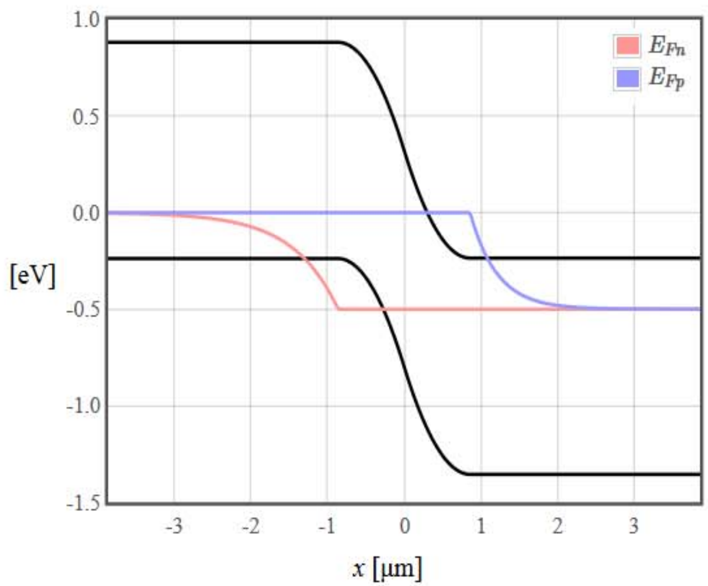
V = -0.5 V Submit

V

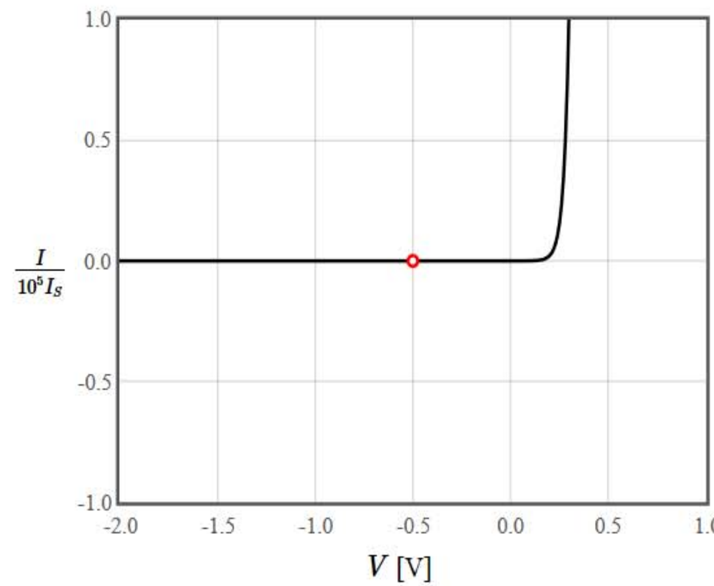
$E_g = 1.12$ eV $W = 1.72$ µm $x_p = -0.861$ µm $x_n = 0.861$ µm $V_{bi} = 0.618$ V $C_j = 6.17$ nF/cm²

$D_p = 12.4$ cm²/s $D_n = 34.9$ cm²/s $L_p = 0.352$ µm $L_n = 0.591$ µm

Band diagram



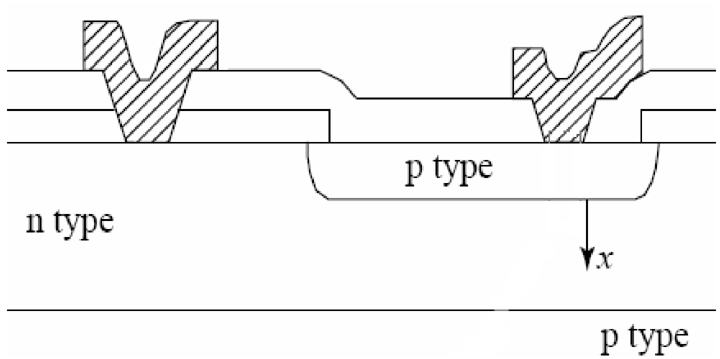
Current-Voltage Characteristics



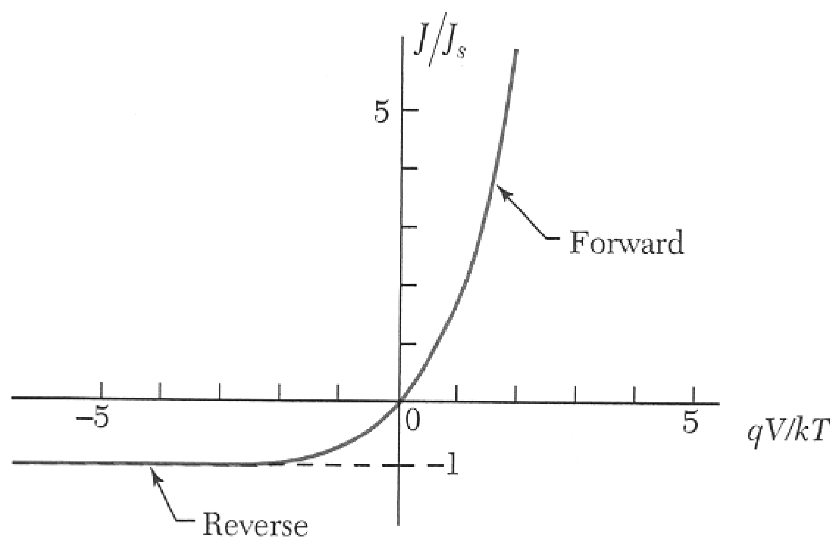
Charge density

Electric field

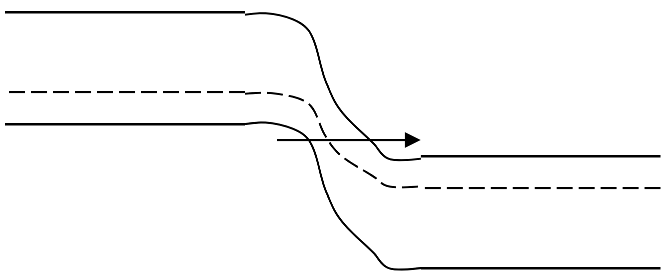
Diode



$$I = I_s\left(\exp\left(\frac{eV}{k_B T}\right) - 1\right)$$

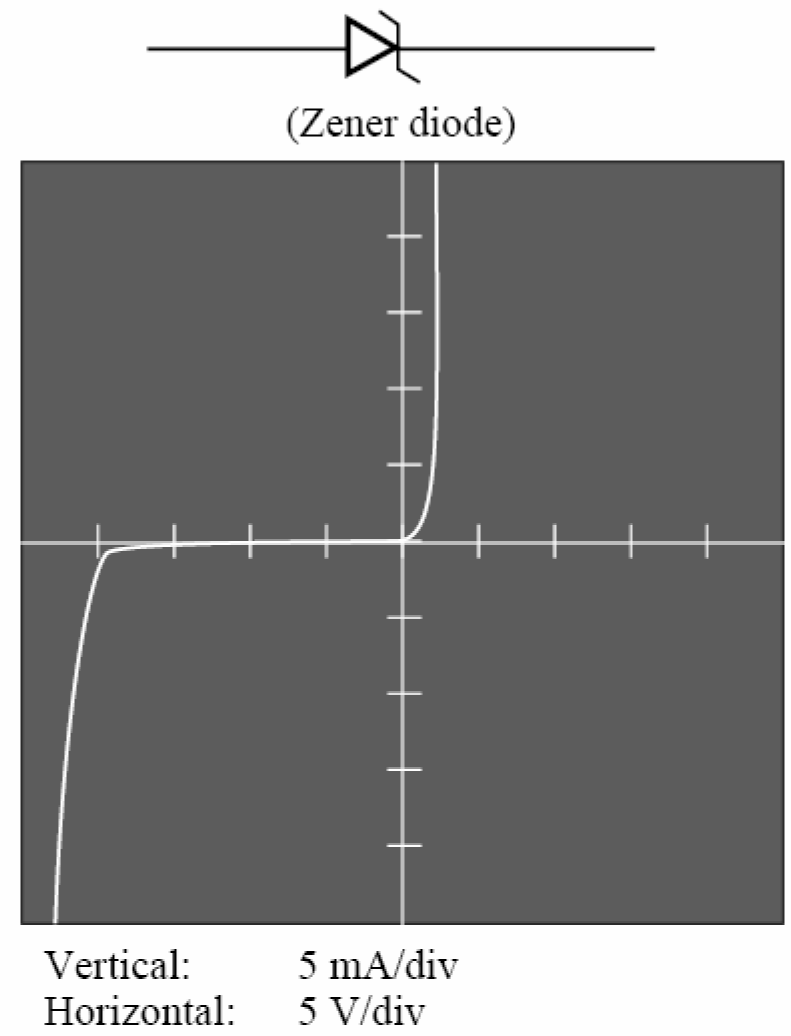


Zener tunneling

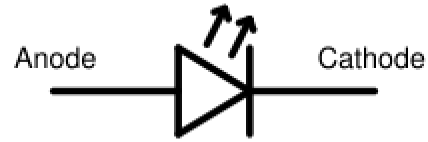


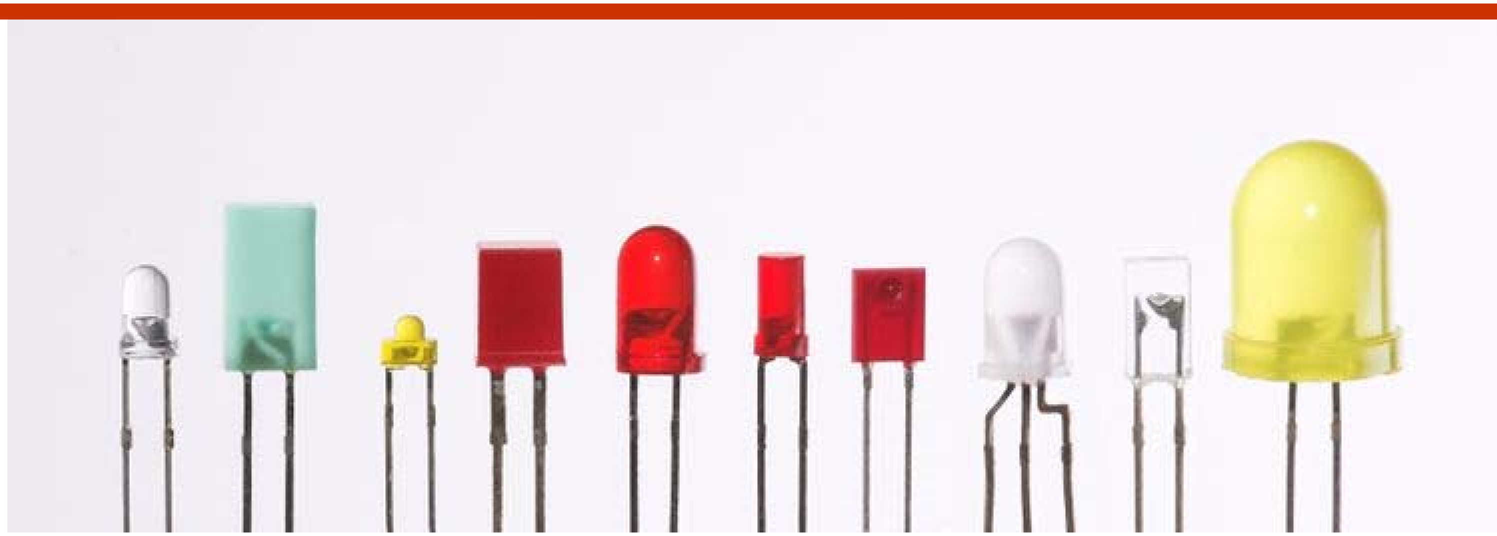
Electrons tunnel from valence band to conduction band

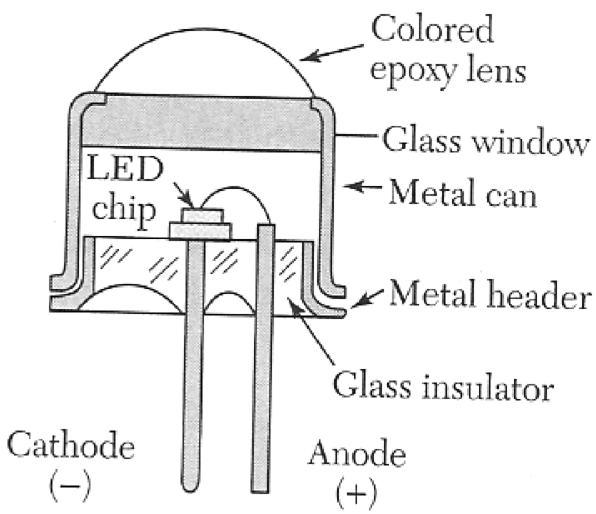
Occurs at high doping

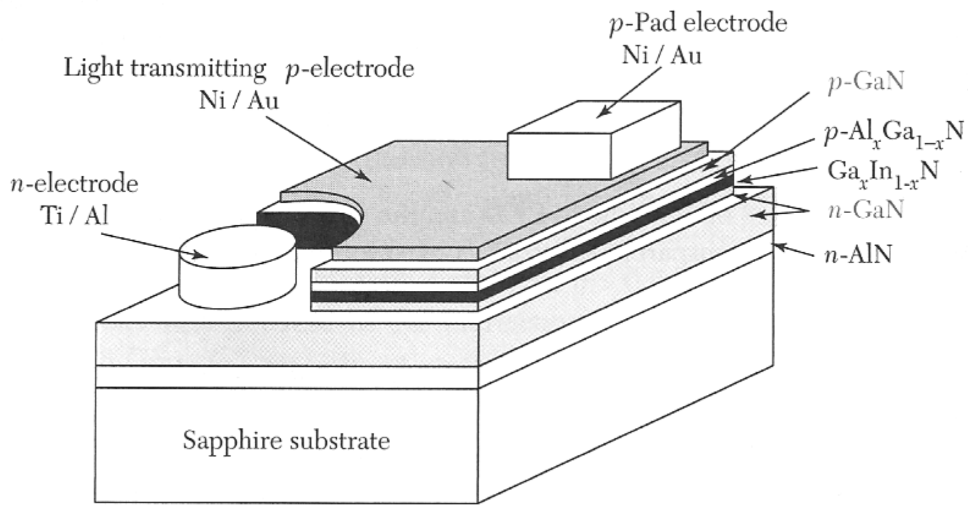


Light emitting diodes



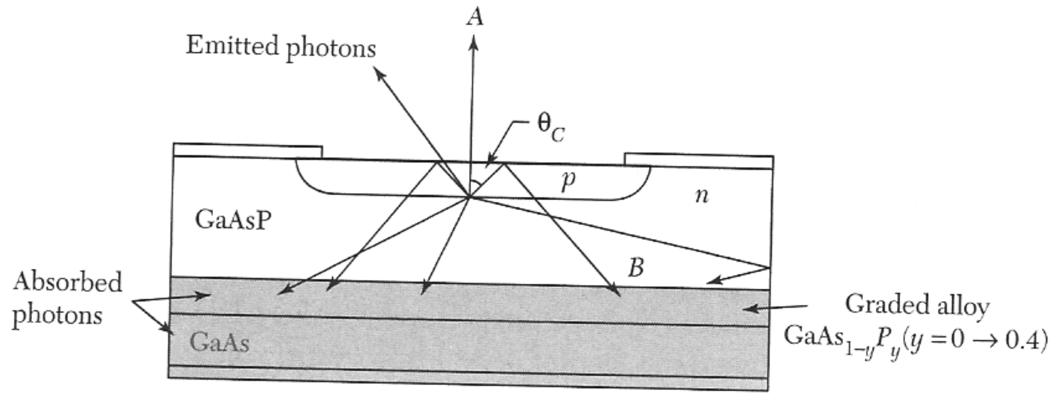




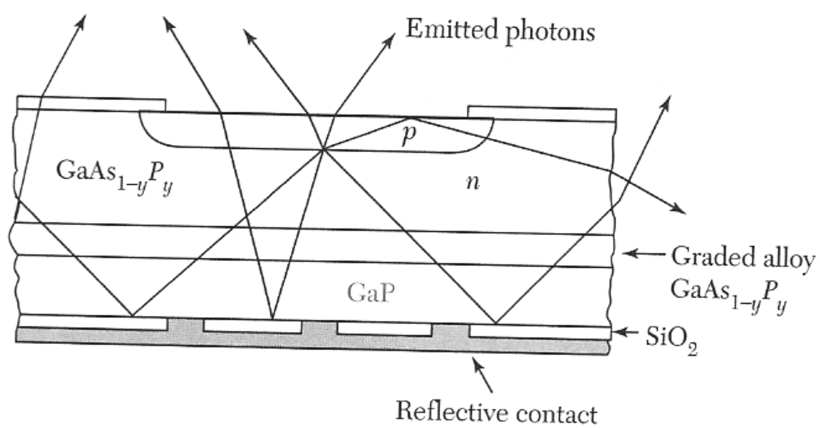


Solid state lighting is efficient.

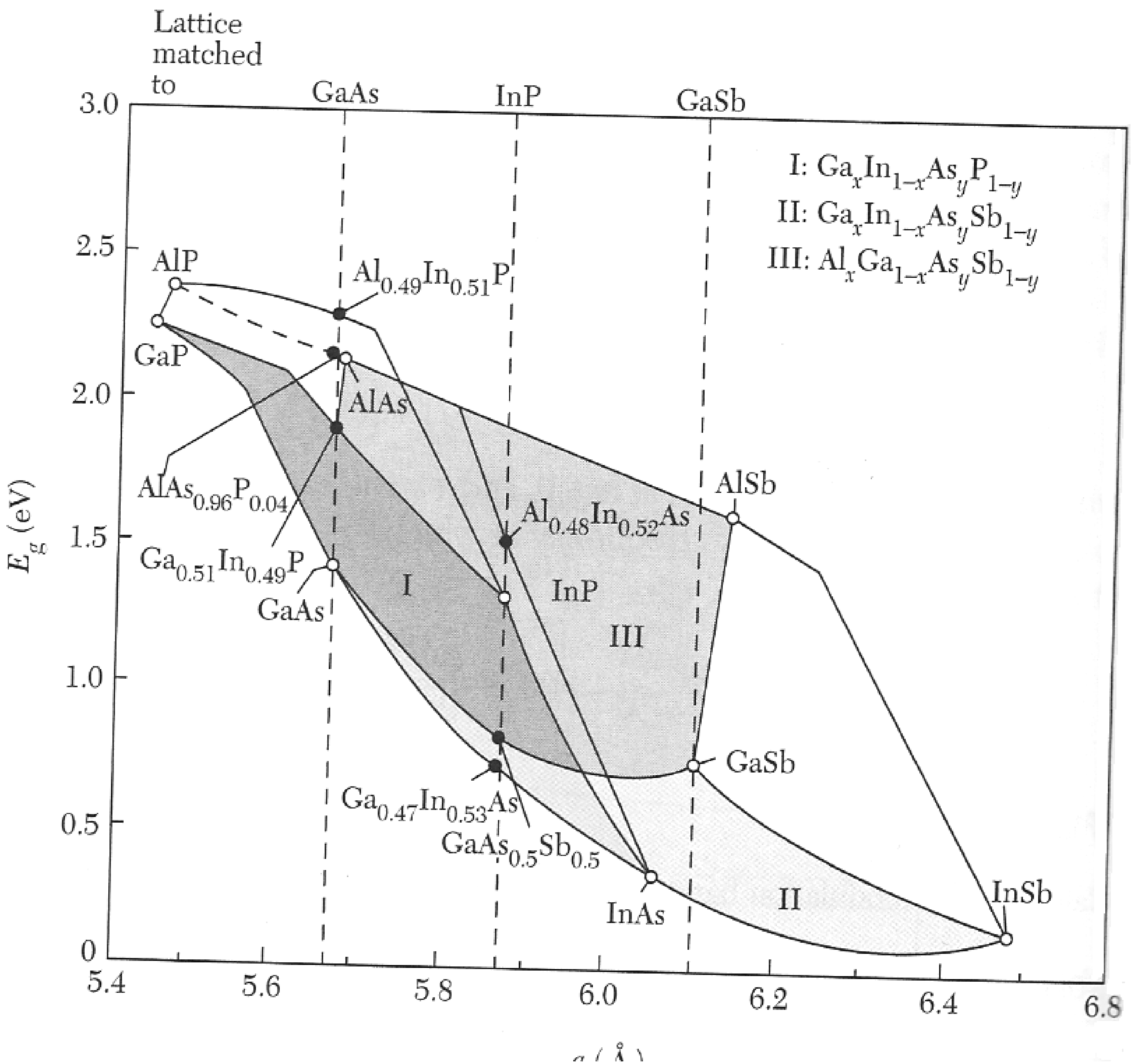
Light emitting diodes



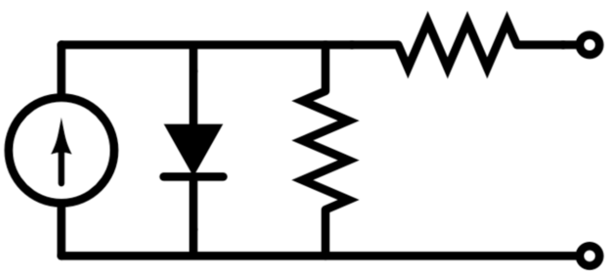
absorption
reflection
total internal reflection



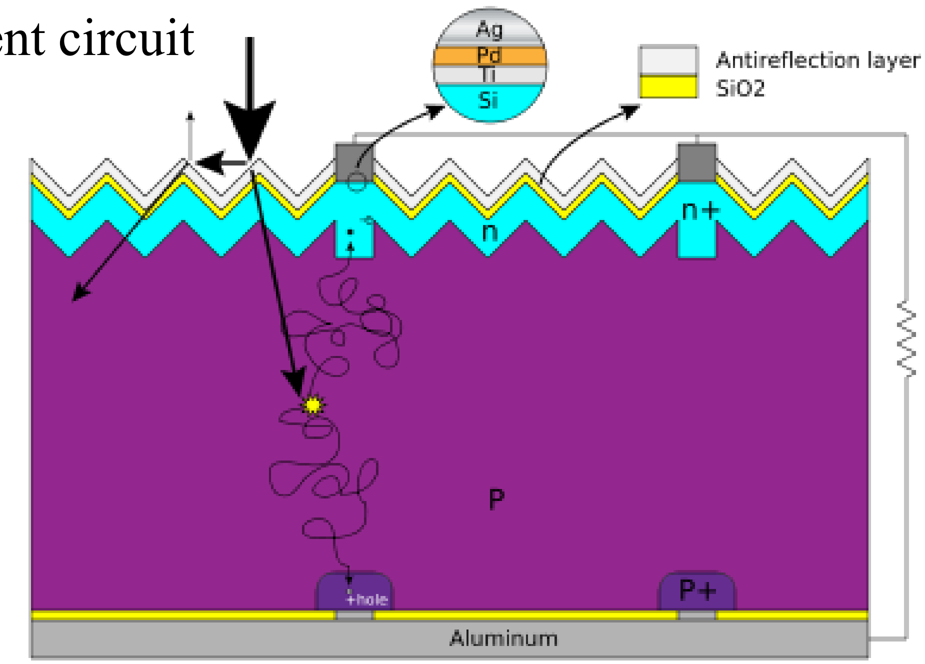
Electrons and holes are injected into the depletion region by forward biasing the junction. The electrons fall in the holes. For direct bandgap semiconductors, photons are emitted. For indirect bandgap semiconductors, phonons are emitted.

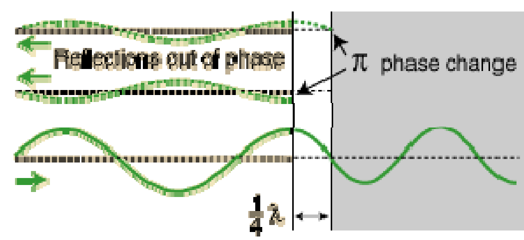

Lattice matched to
GaAs
InP
GaSb
I: $Ga_xIn_{1-x}As_yP_{1-y}$
II: $Ga_xIn_{1-x}As_ySb_{1-y}$
III: $Al_xGa_{1-x}As_ySb_{1-y}$
AlP
GaP
$Al_{0.49}In_{0.51}P$
AlAs
$AlAs_{0.96}P_{0.04}$
$Ga_{0.51}In_{0.49}P$
GaAs
I
$Al_{0.48}In_{0.52}As$
InP
III
AlSb
GaSb
$Ga_{0.47}In_{0.53}As$
$GaAs_{0.5}Sb_{0.5}$
InAs
II
InSb
E_g (eV)
3.0
2.5
2.0
1.5
1.0
0.5
0
5.4
5.6
5.8
6.0
6.2
6.4
6.8

Solar cell

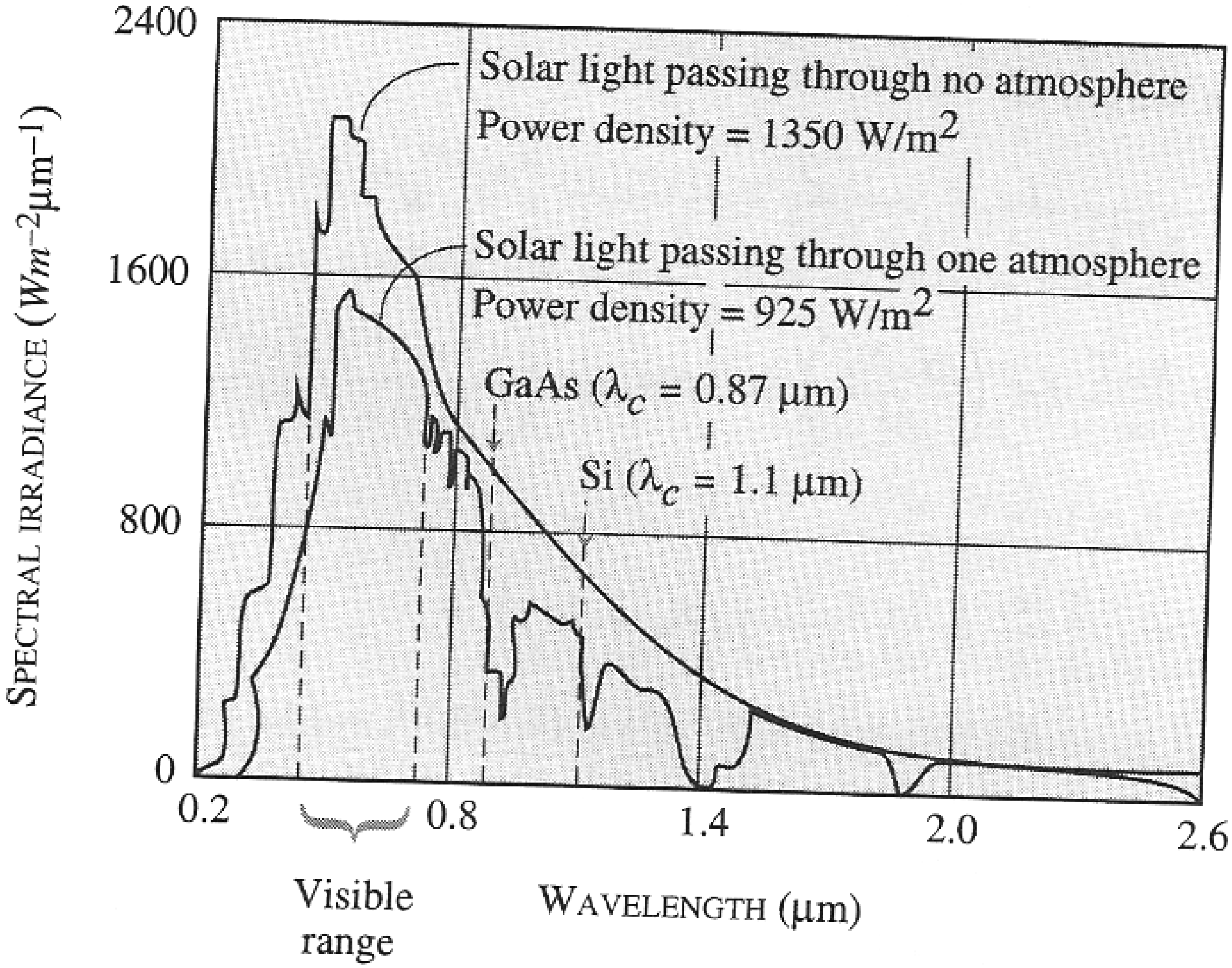


Equivalent circuit



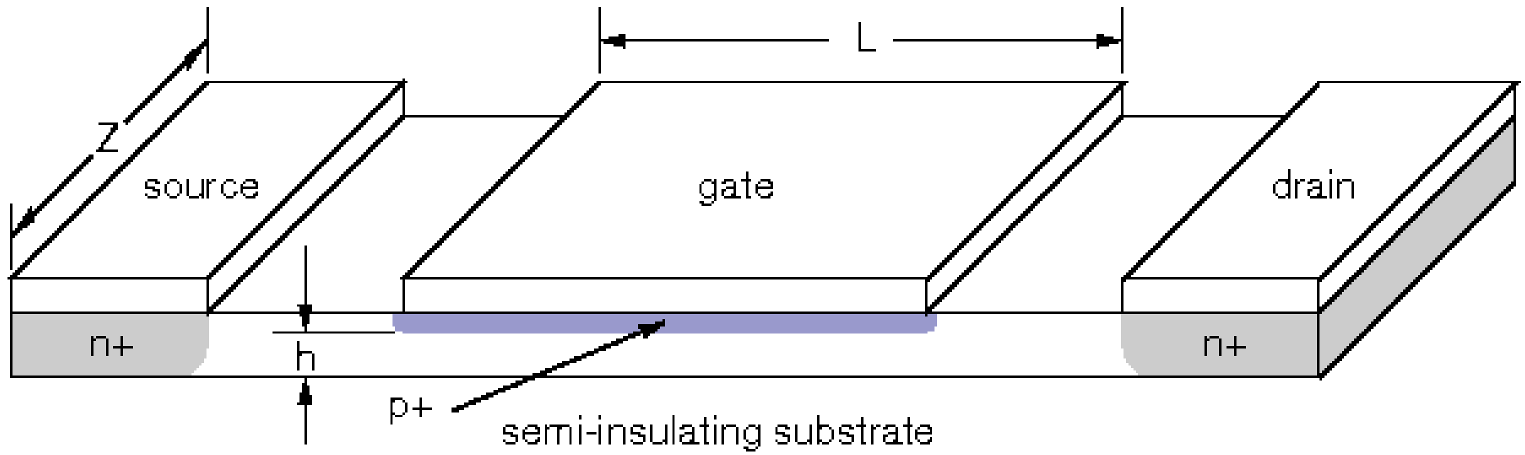


Solar spectrum



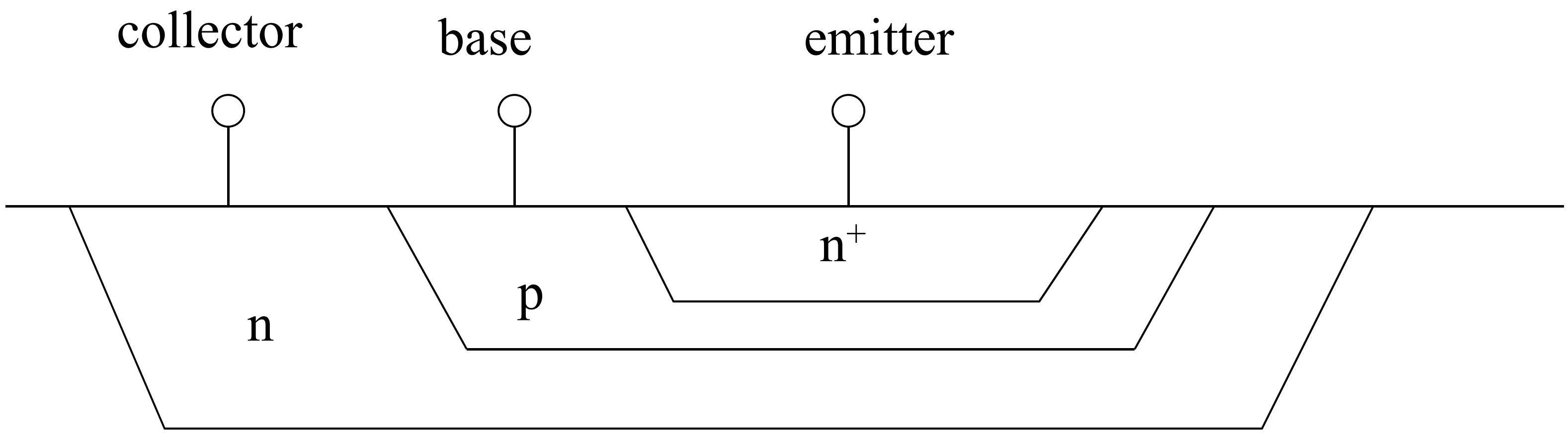
JFETs

Junction Field Effect Transistors



low noise

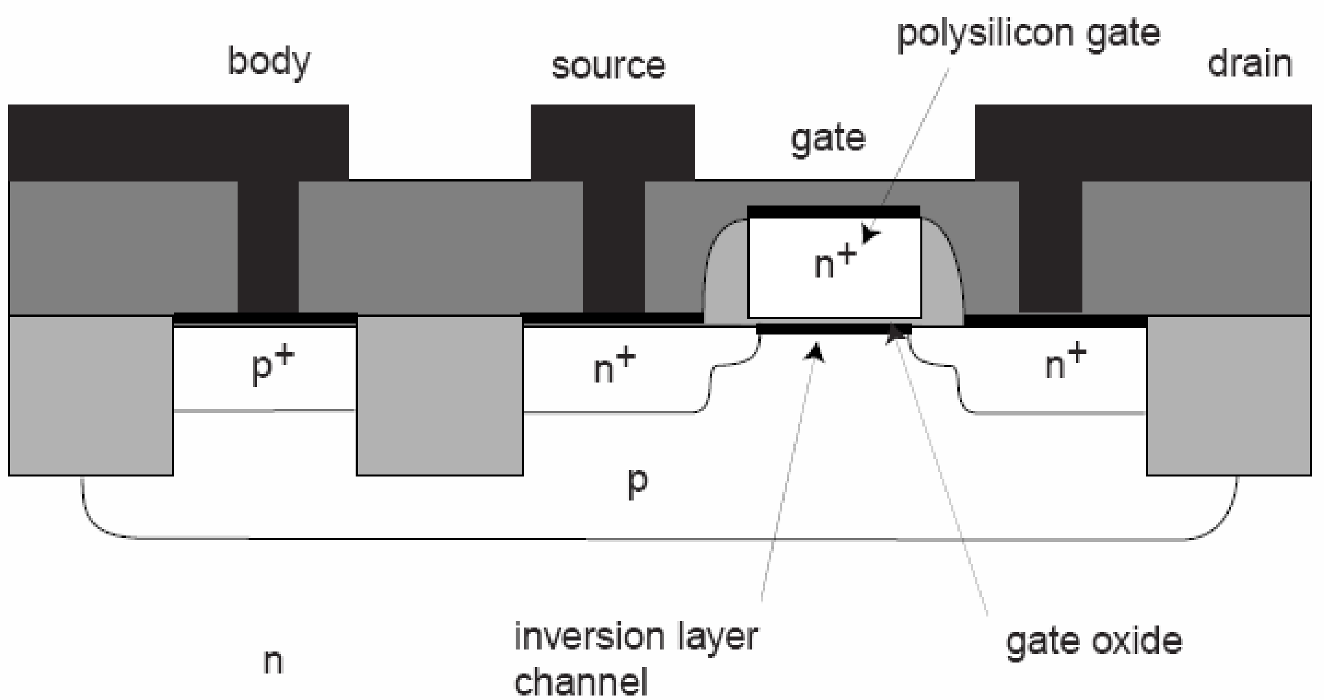
Bipolar transistor

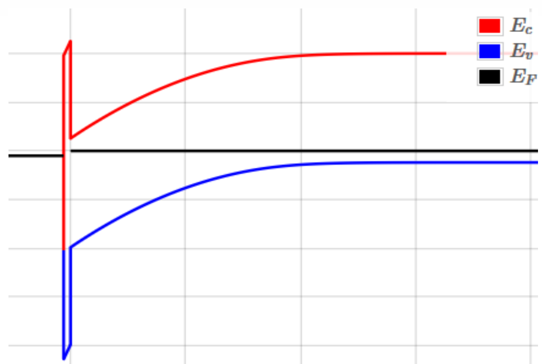


lightly doped p substrate

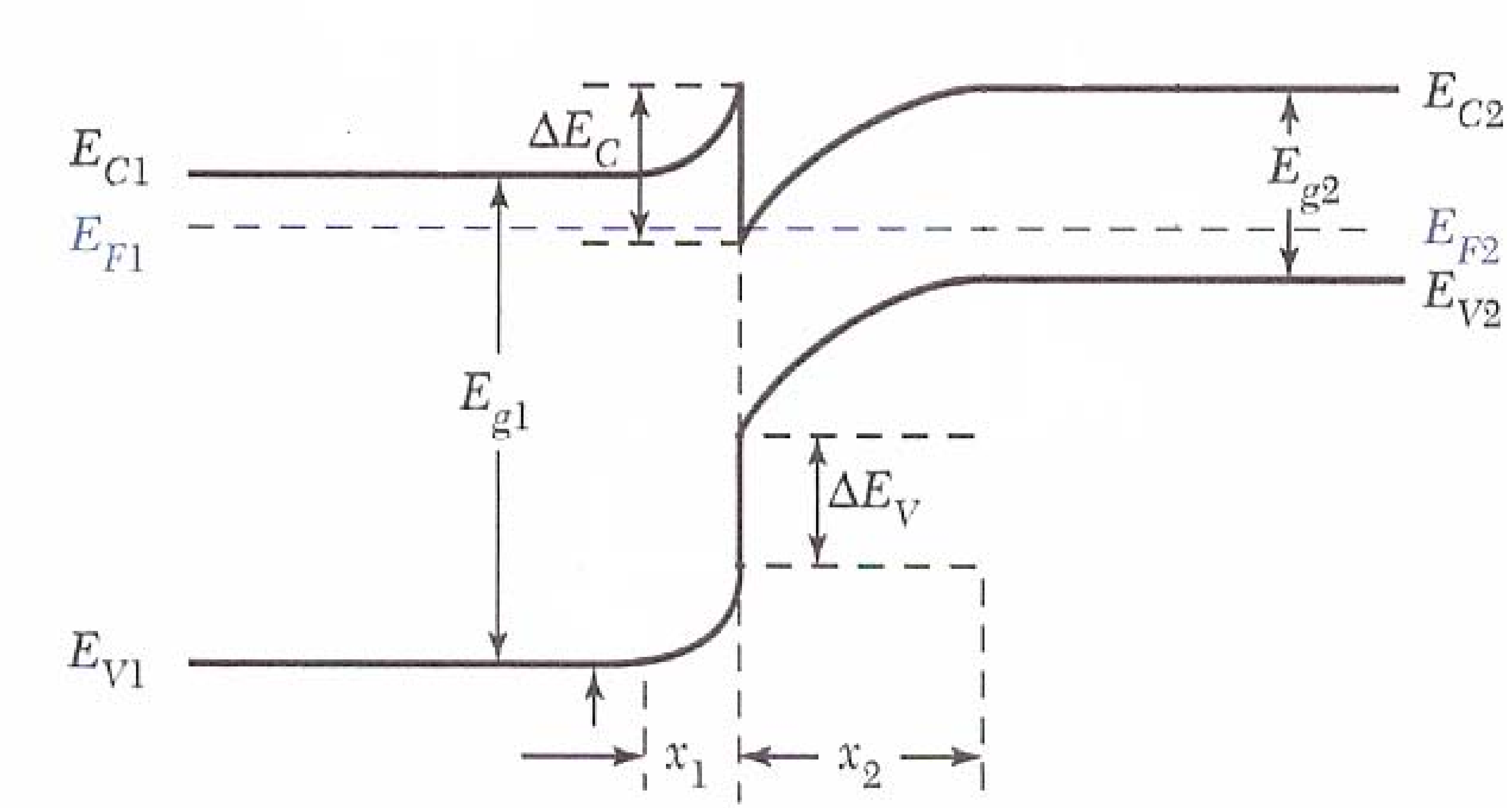
MOSFETs

Metal-oxide semiconductor field effect transistors





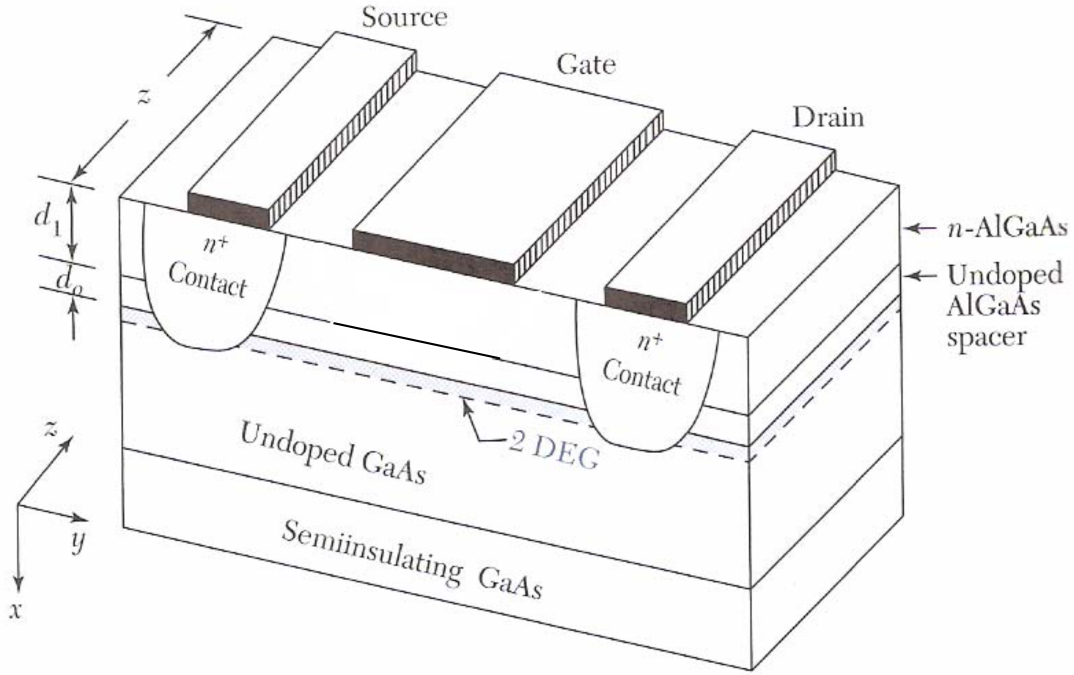
Heterojunctions

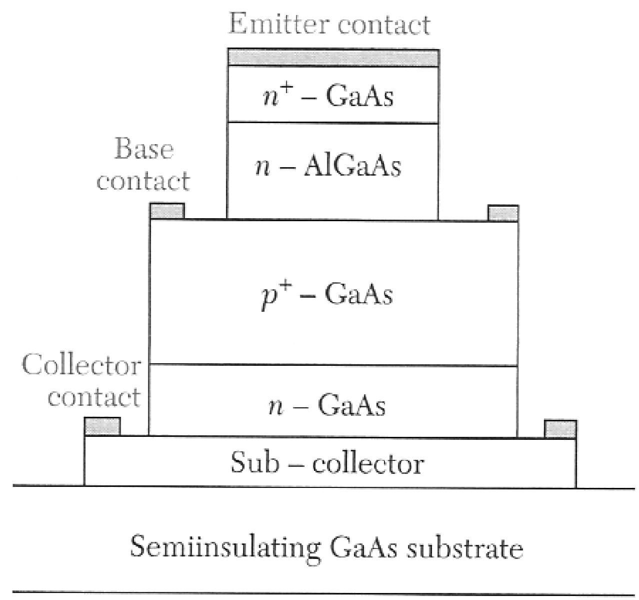


Quantum hall effect
Quantized conductance
HBTs
HEMTs

HEMT High electron mobility transistor

HBT Hetero junction bipolar transistor

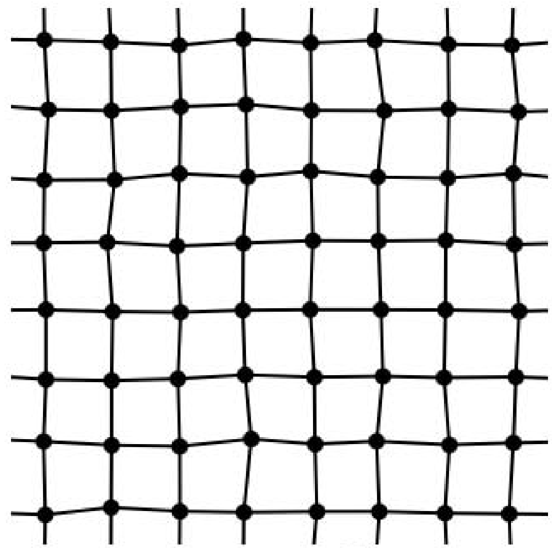




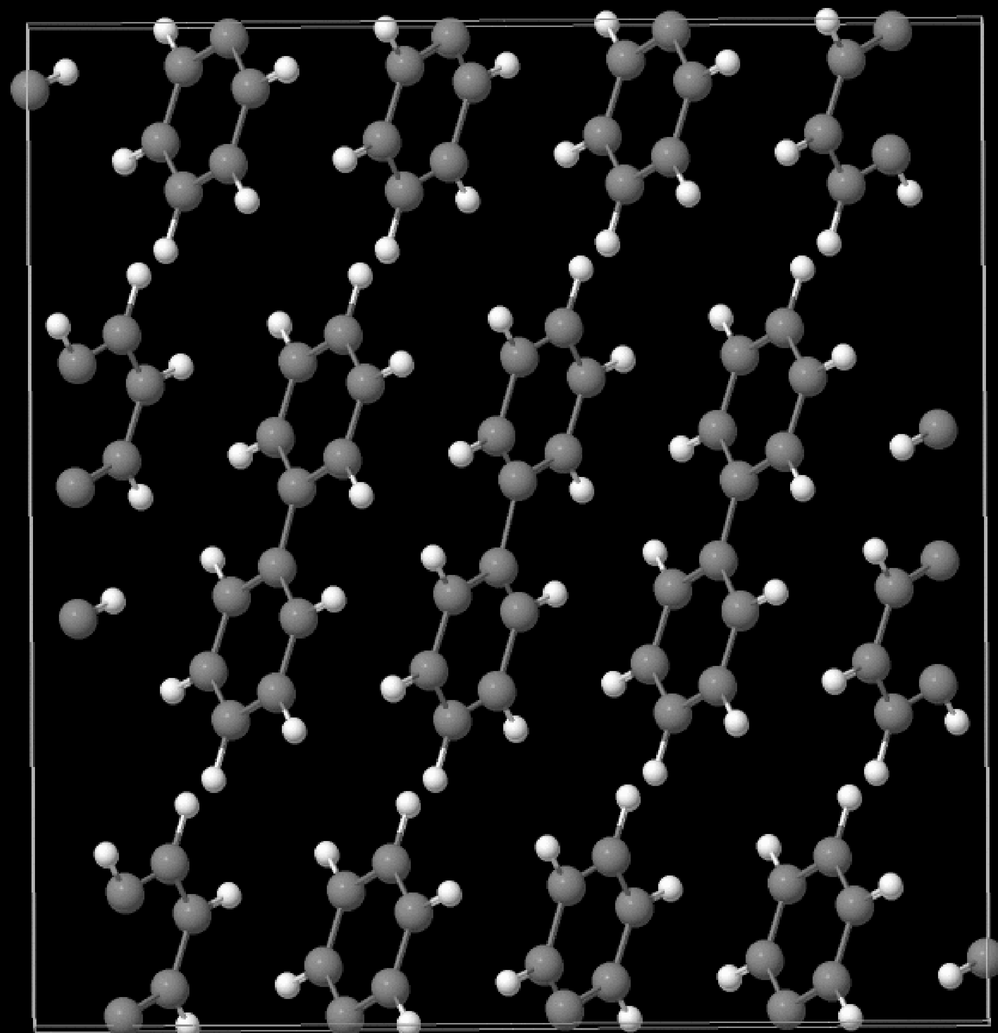
Phonons

Normal Modes and Phonons

At finite temperatures, the atoms in a crystal vibrate. In the simulation below, the atoms move randomly around their equilibrium positions.



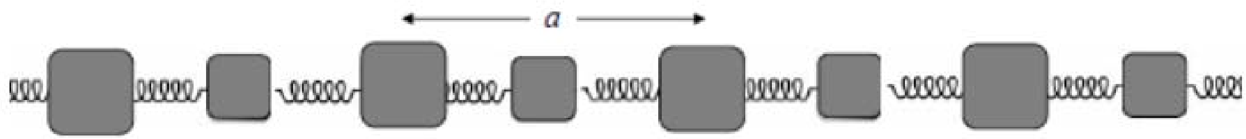
T = 300 K - +



Natalia Bedoya

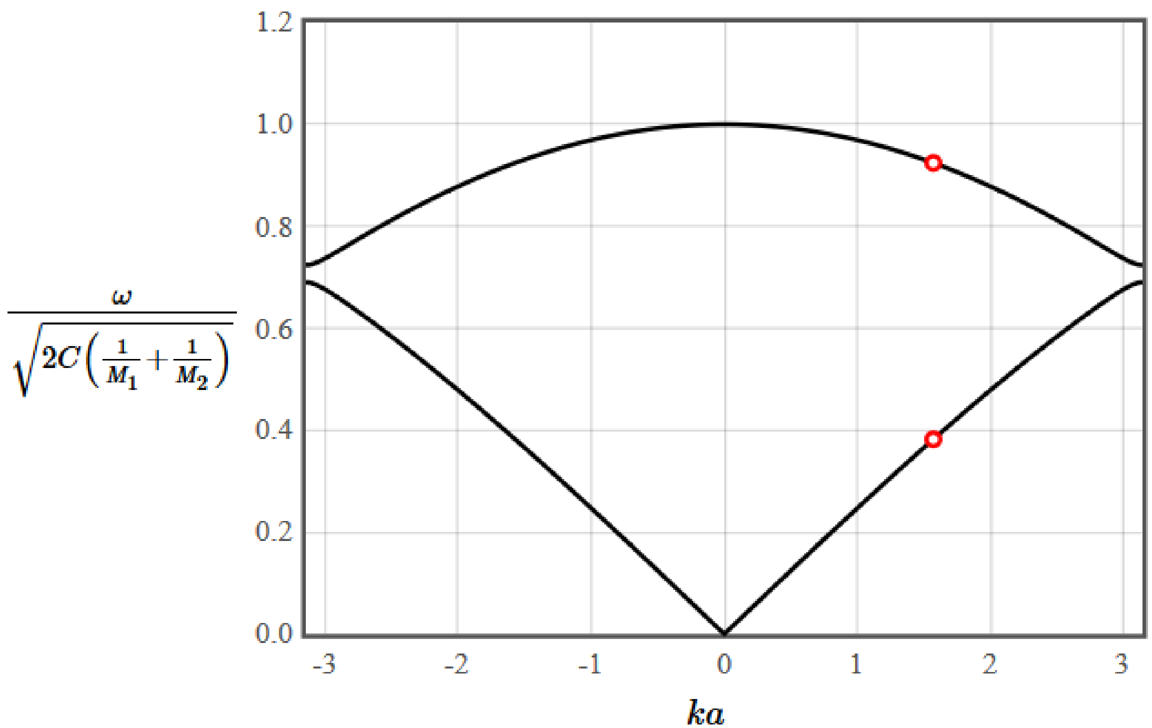
In a normal mode, all of the atoms oscillate at the same frequency.

1-d chain of atoms with two different masses



$$M_1 \frac{d^2 u_l}{dt^2} = C(v_{l-1} - 2u_l + v_l)$$

$$M_2 \frac{d^2 v_l}{dt^2} = C(u_l - 2v_l + u_{l+1})$$



Phonons

N_{atom} atoms in crystal
$3N_{atom}$ normal modes
p atoms in the basis
N_{atom}/p unit cells
N_{atom}/p translational symmetries
N_{atom}/p k-vectors
$3p$ modes for every k vector
3 acoustic branches and $3p$-3 optical branches

Normal modes are eigenfunctions of T

$$u_{lmn}^{x} = u_{\vec{k}}^{x} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

$$u_{lmn}^{y} = u_{\vec{k}}^{y} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

$$u_{lmn}^{z} = u_{\vec{k}}^{z} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

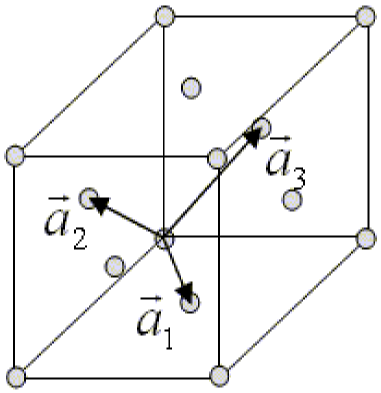
These are eigenfunctions of T.

$$T_{pqr}u_{lmn}^{x} = u_{\vec{k}}^{x} \exp\left(i\left(l\vec{k}\cdot\left(\vec{a}_1 + p\vec{a}_1\right) + m\vec{k}\cdot\left(\vec{a}_2 + q\vec{a}_2\right) + n\vec{k}\cdot\left(\vec{a}_3 + r\vec{a}_3\right) - \omega t\right)\right)$$

$$= \exp\left(i\left(lp\vec{k}\cdot\vec{a}_1 + qm\vec{k}\cdot\vec{a}_2 + rn\vec{k}\cdot\vec{a}_3\right)\right) u_{\vec{k}}^{x} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

$$= \exp\left(i\left(lp\vec{k}\cdot\vec{a}_1 + qm\vec{k}\cdot\vec{a}_2 + rn\vec{k}\cdot\vec{a}_3\right)\right) u_{lmn}^{x}$$

fcc



$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} \qquad \vec{b}_1 = \frac{2\pi}{a}\left(\hat{k}_x + \hat{k}_y - \hat{k}_z\right)$$

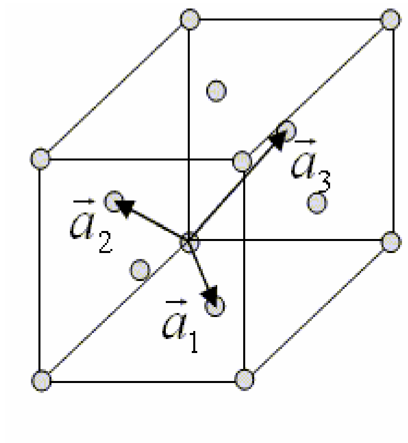
$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z} \qquad \vec{b}_2 = \frac{2\pi}{a}\left(\hat{k}_x - \hat{k}_y + \hat{k}_z\right)$$

$$\vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z} \qquad \vec{b}_3 = \frac{2\pi}{a}\left(-\hat{k}_x + \hat{k}_y + \hat{k}_z\right)$$

$$\begin{aligned} m\frac{d^2u^x_{lmn}}{dt^2} = \frac{C}{2}\Big[& \left(u^x_{l+1mn} - u^x_{lmn}\right) + \left(u^x_{l-1mn} - u^x_{lmn}\right) + \left(u^x_{lm+1n} - u^x_{lmn}\right) + \left(u^x_{lm-1n} - u^x_{lmn}\right) \\ & + \left(u^x_{l+1mn-1} - u^x_{lmn}\right) + \left(u^x_{l-1mn+1} - u^x_{lmn}\right) + \left(u^x_{lm+1n-1} - u^x_{lmn}\right) + \left(u^x_{lm-1n+1} - u^x_{lmn}\right) \\ & + \left(u^y_{l+1mn} - u^y_{lmn}\right) + \left(u^y_{l-1mn} - u^y_{lmn}\right) - \left(u^y_{lm+1n-1} - u^y_{lmn}\right) - \left(u^y_{lm-1n+1} - u^y_{lmn}\right) \\ & + \left(u^z_{lm+1n} - u^z_{lmn}\right) + \left(u^z_{lm-1n} - u^z_{lmn}\right) - \left(u^z_{l+1mn-1} - u^z_{lmn}\right) - \left(u^z_{l-1mn+1} - u^z_{lmn}\right)\Big] \end{aligned}$$

and similar expressions for the *y* and *z* motion

fcc



$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

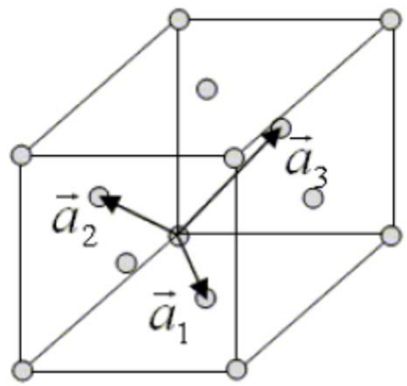
Substitute the eigenfunctions of *T* into Newton's laws.

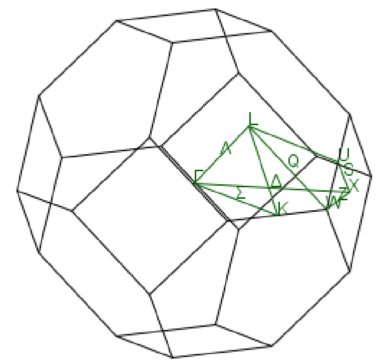
$$u_{lmn}^{x} = u_{\vec{k}}^{x}\exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3\right)\right) = u_{\vec{k}}^{x}\exp\left(i\left(\frac{(l+m)k_xa}{2} + \frac{(l+n)k_ya}{2} + \frac{(m+n)k_za}{2}\right)\right).$$

$$\begin{vmatrix} 4-\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)-\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)-\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right)-\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right) & -\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right) \\ -\cos\left(\frac{k_xa}{2}+\frac{k_ya}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_ya}{2}\right) & 4-\cos\left(\frac{k_ya}{2}+\frac{k_xa}{2}\right)-\cos\left(\frac{k_ya}{2}+\frac{k_za}{2}\right)-\cos\left(\frac{k_ya}{2}-\frac{k_xa}{2}\right)-\cos\left(\frac{k_ya}{2}-\frac{k_za}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_ya}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_ya}{2}-\frac{k_za}{2}\right) \\ -\cos\left(\frac{k_xa}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_xa}{2}-\frac{k_za}{2}\right) & -\cos\left(\frac{k_ya}{2}+\frac{k_za}{2}\right)+\cos\left(\frac{k_ya}{2}-\frac{k_za}{2}\right) & 4-\cos\left(\frac{k_za}{2}+\frac{k_xa}{2}\right)-\cos\left(\frac{k_za}{2}+\frac{k_ya}{2}\right)-\cos\left(\frac{k_za}{2}-\frac{k_xa}{2}\right)-\cos\left(\frac{k_za}{2}-\frac{k_ya}{2}\right)-\frac{m\omega^2}{\sqrt{2}C} \end{vmatrix} = 0$$

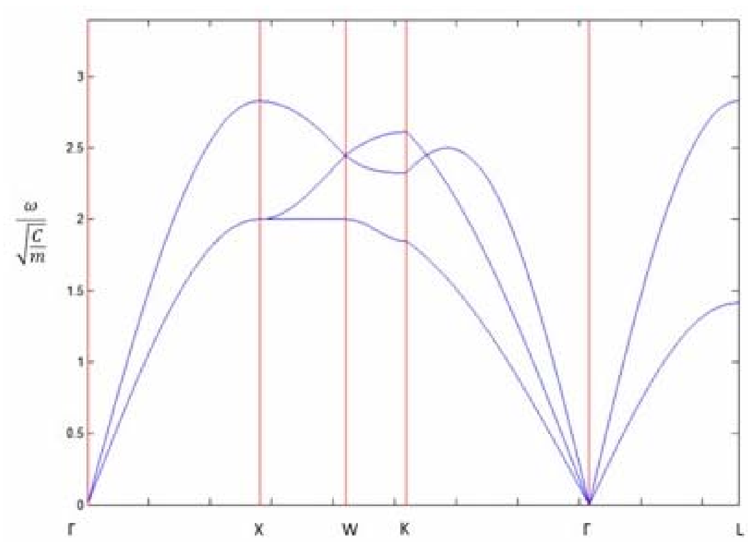
http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/fcc/fcc.html

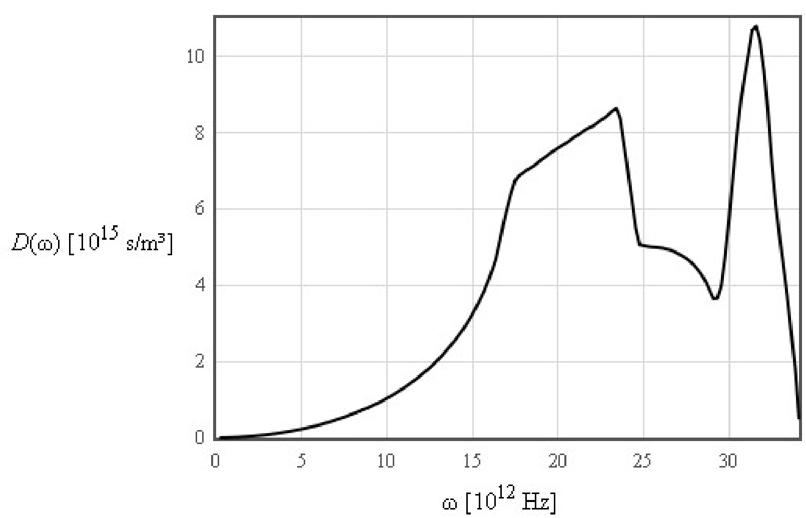
fcc phonons



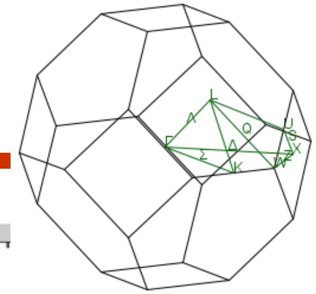


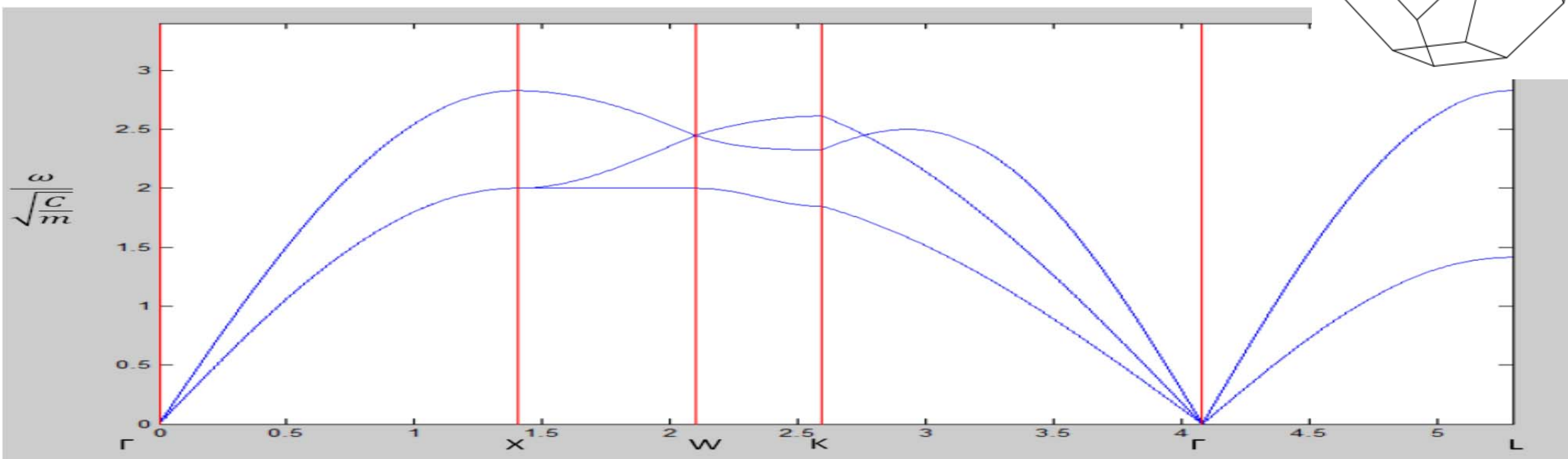
3N degrees of freedom





Phonon dispersion Au





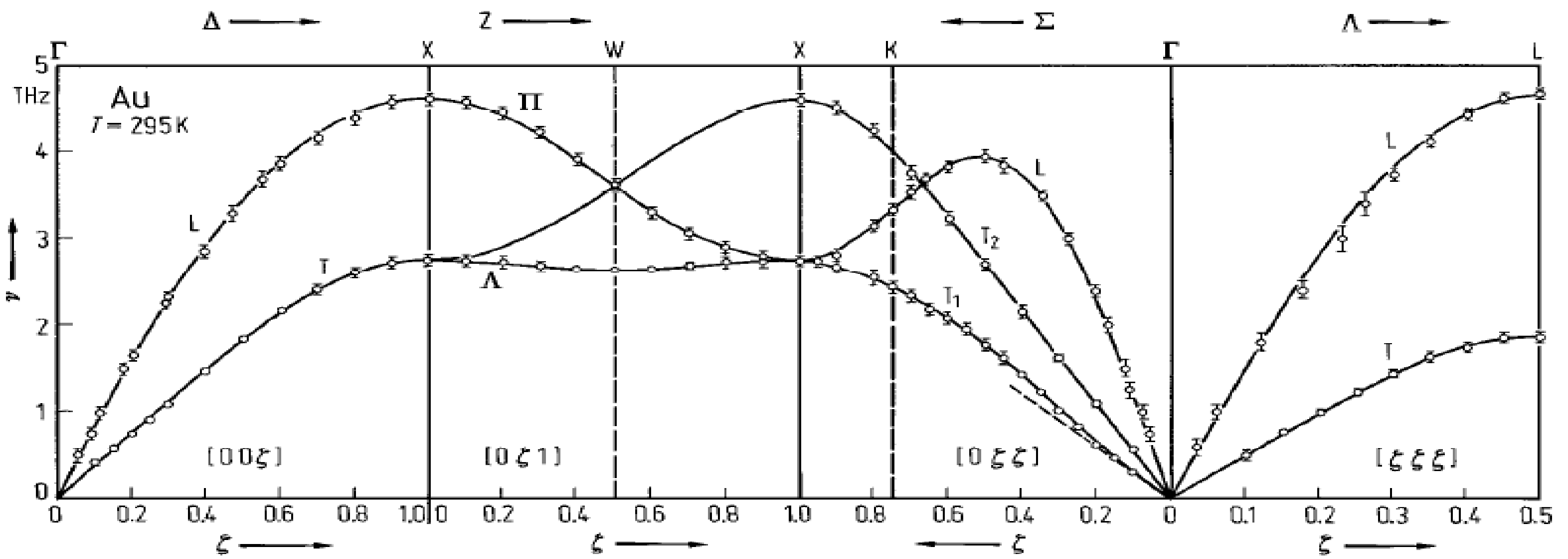
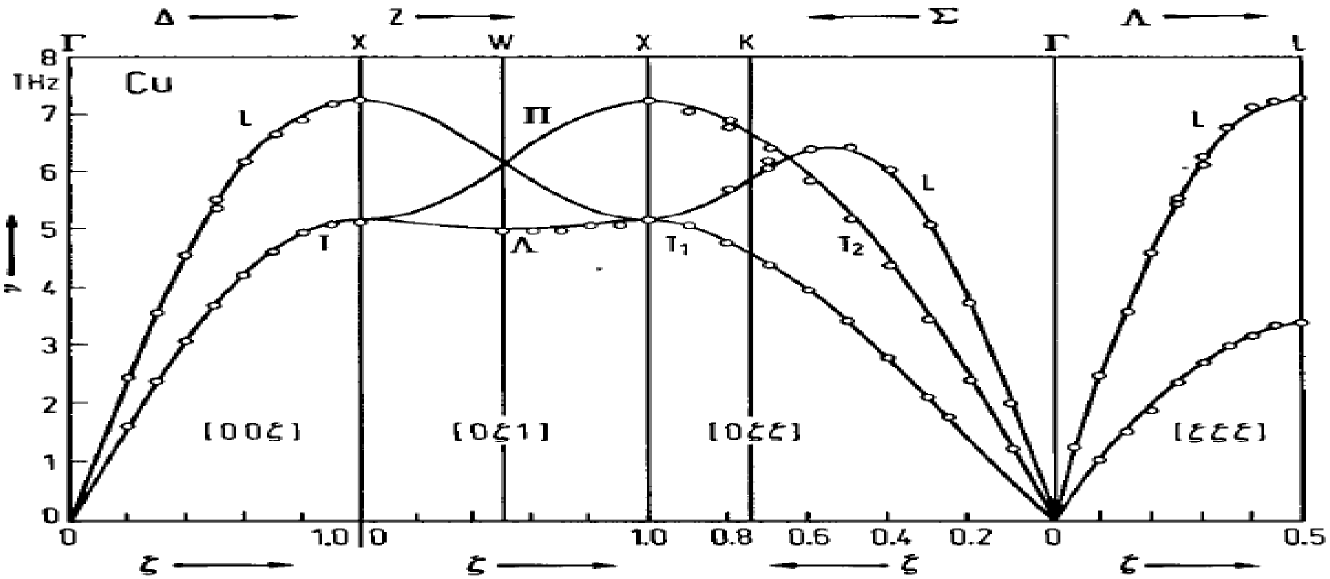


Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the [0ζζ] T_1 branch.

From Springer Materials: Landholt Boernstein Database

Materials with the same crystal structure will have similar phonon dispersion relations



Cu

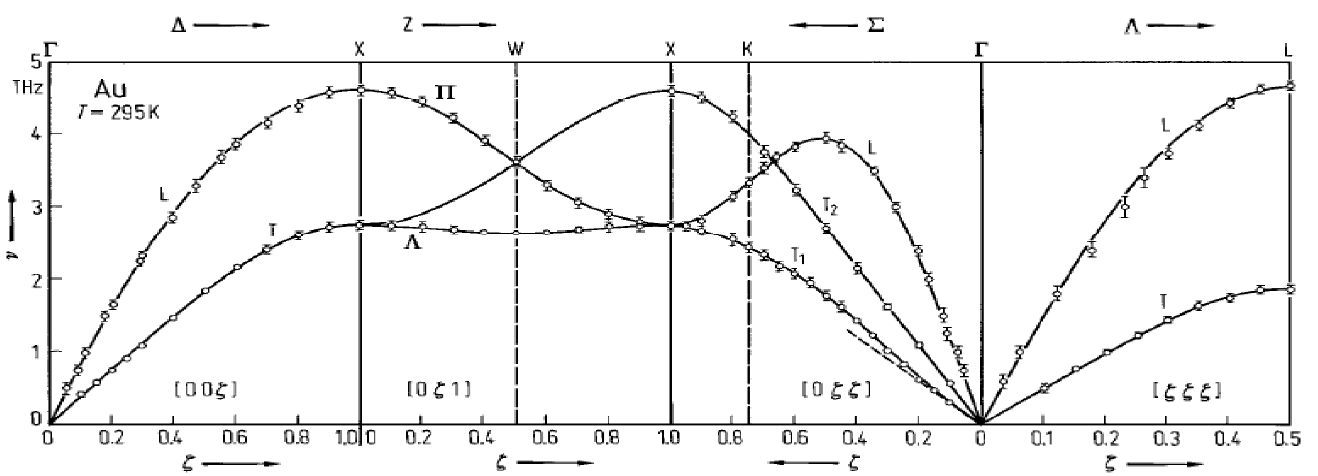
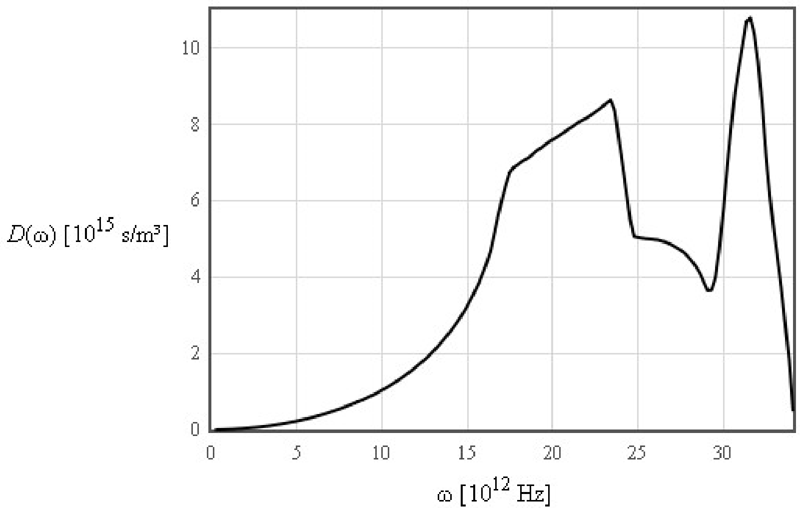


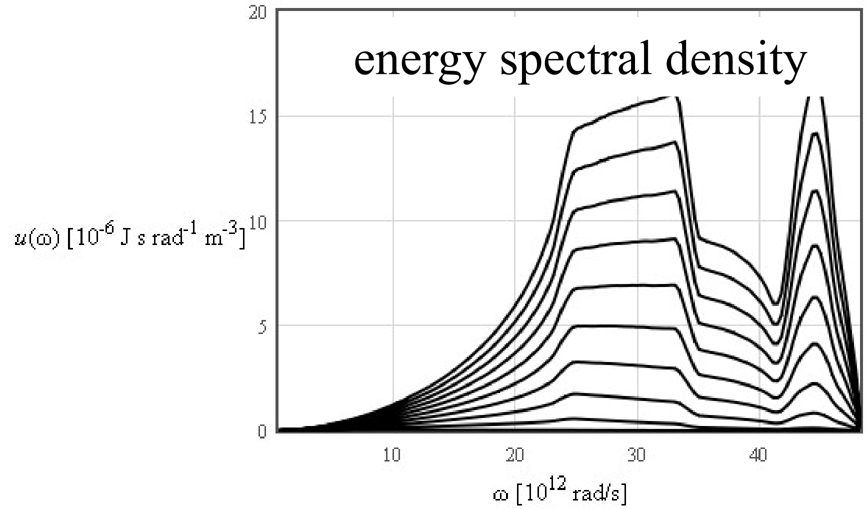
Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the [0ζζ] T_1 branch.

Au

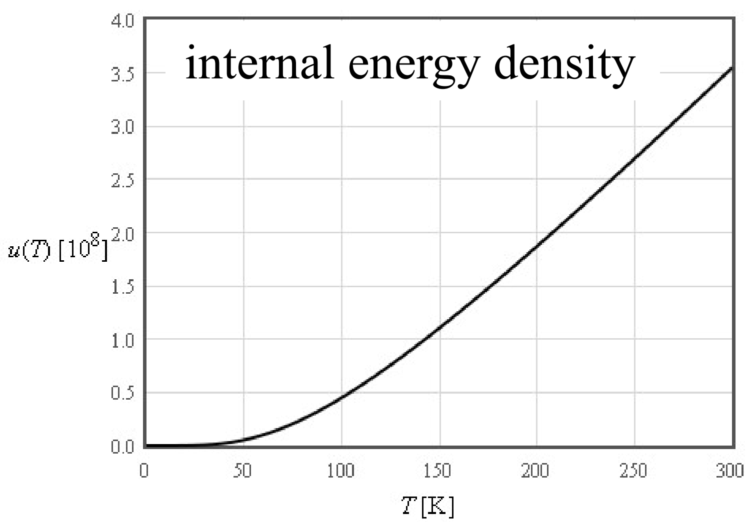
fcc phonons



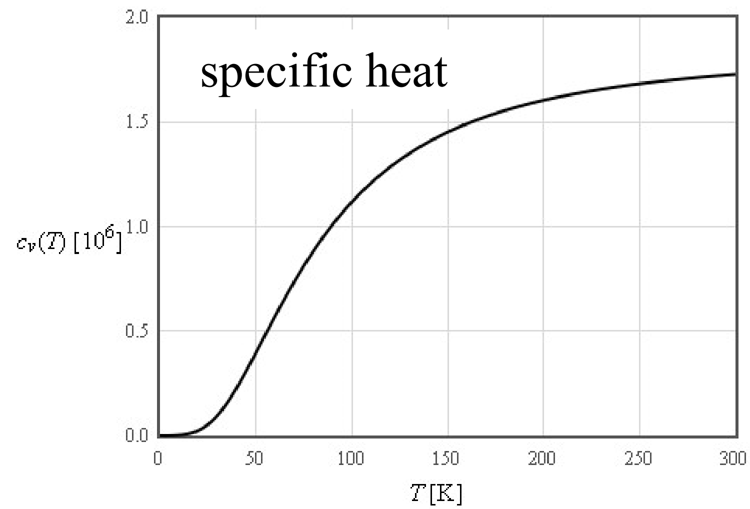
$D(\omega)$ [10^{15} s/m³]
ω [10^{12} Hz]



energy spectral density
$u(\omega)$ [10^{-6} J s rad^{-1} m^{-3}]
ω [10^{12} rad/s]

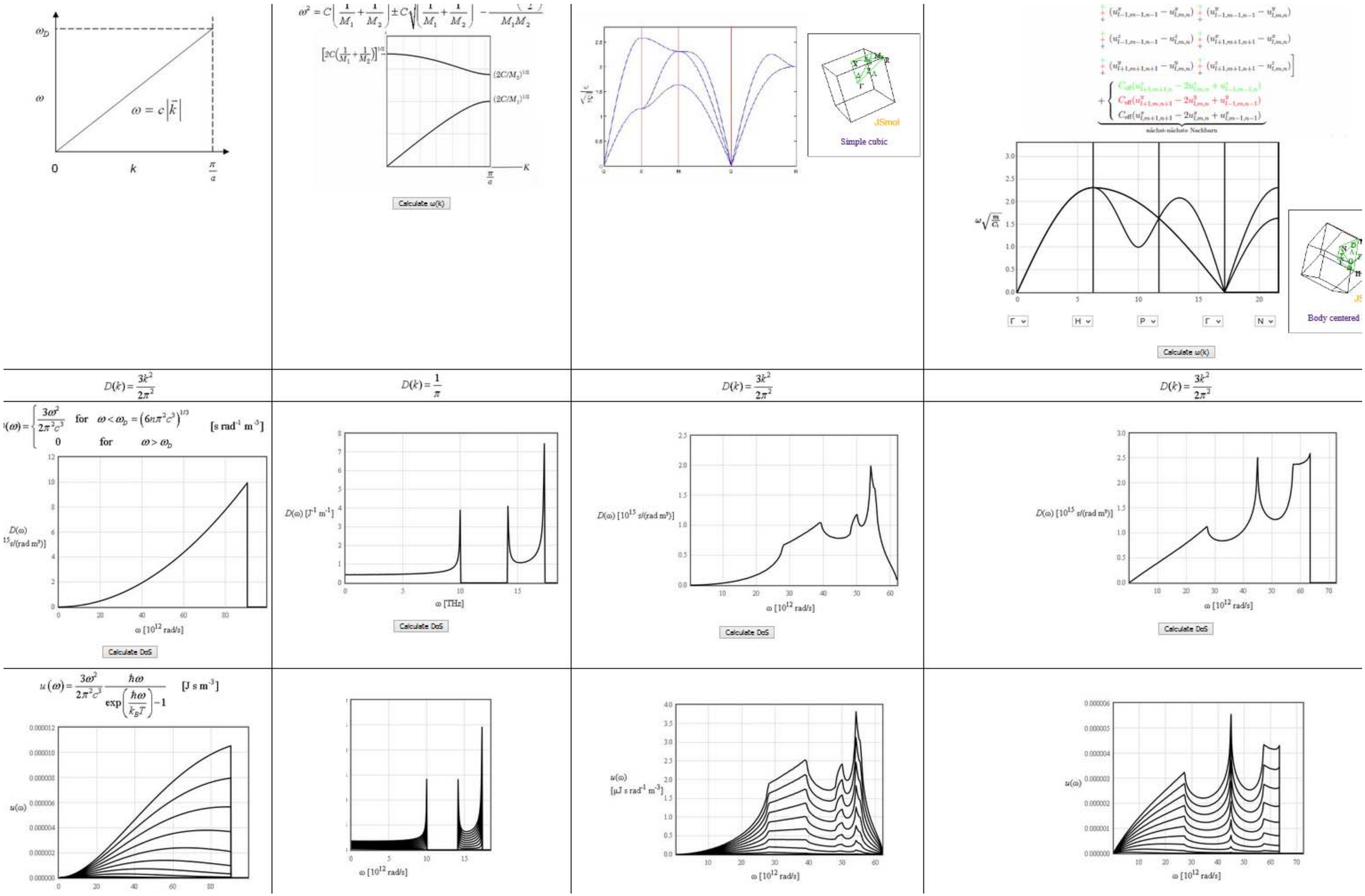


internal energy density
$u(T)$ [10^8]
T [K]



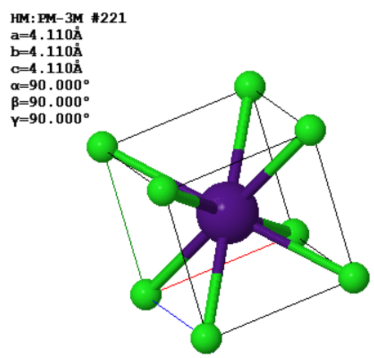
specific heat
$c_V(T)$ [10^6]
T [K]

Table summarizing the thermodynamic properties of phonons



http://lampx.tugraz.at/~hadley/ss1/phonons/phonontable.html

Phonon dispersion of CsCl



Conventional unit cell | Asymmetric unit | 2 x 2 x 2
3 x 3 x 3 | 5 x 5 x 5
Ball and Stick | Spacefill
Label Atoms | Atom Labels Off

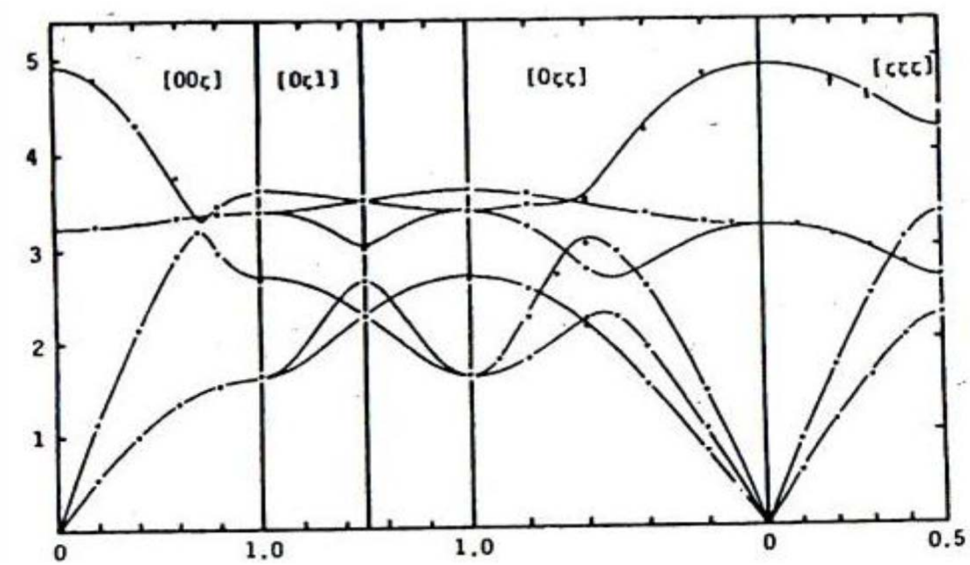
H: 1 K: 0 L: 0
show HKL plane | hide HKL plane
draw atoms in HKL plane
Thickness of HKL planes:
0 Å — 10 Å

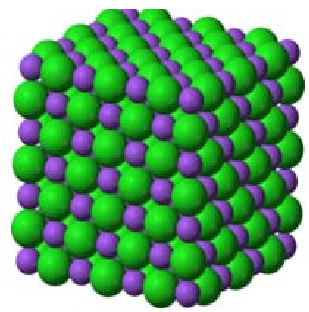
The conventional unit cell is a cube with sides of *a*. There is one Cs atom and one Cl atom in the conventional unit cell. The Bravais lattice is simple cubic.

JSmol

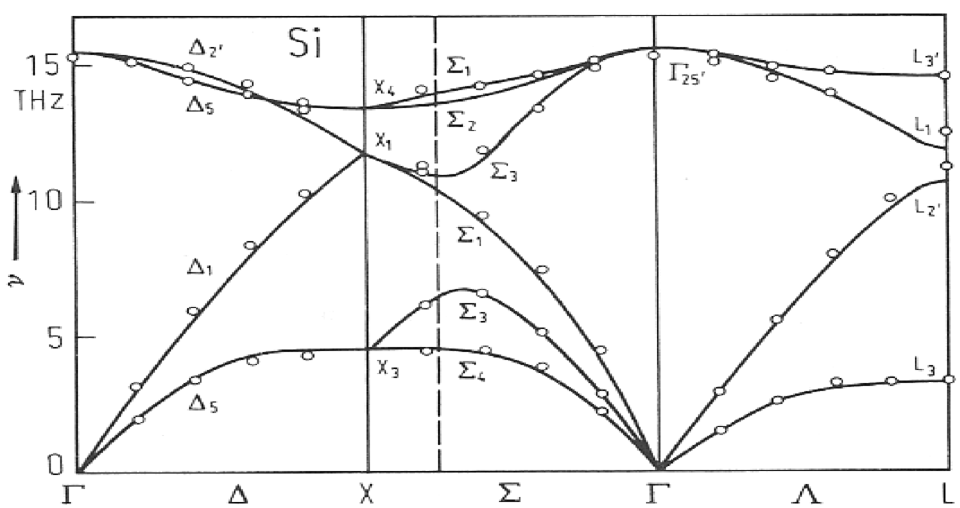
$$
\begin{aligned}
M_{\text{Cs}}\frac{d^2u^x_{lmn}}{dt^2} = \frac{C_{\text{Cs-Cl}}}{3}\Big[&+(v^x_{lmn}-u^x_{lmn})+(v^y_{lmn}-u^y_{lmn})+(v^z_{lmn}-u^z_{lmn})\\
&+(v^x_{(l-1)mn}-u^x_{lmn})-(v^y_{(l-1)mn}-u^y_{lmn})-(v^z_{(l-1)mn}-u^z_{lmn})\\
&+(v^x_{(l-1)(m-1)n}-u^x_{lmn})+(v^y_{(l-1)(m-1)n}-u^y_{lmn})-(v^z_{(l-1)(m-1)n}-u^z_{lmn})\\
&+(v^x_{l(m-1)n}-u^x_{lmn})-(v^y_{l(m-1)n}-u^y_{lmn})+(v^z_{l(m-1)n}-u^z_{lmn})\\
&+(v^x_{lm(n-1)}-u^x_{lmn})+(v^y_{lm(n-1)}-u^y_{lmn})-(v^z_{lm(n-1)}-u^z_{lmn})\\
&+(v^x_{(l-1)m(n-1)}-u^x_{lmn})-(v^y_{(l-1)m(n-1)}-u^y_{lmn})+(v^z_{(l-1)m(n-1)}-u^z_{lmn})\\
&+(v^x_{(l-1)(m-1)(n-1)}-u^x_{lmn})+(v^y_{(l-1)(m-1)(n-1)}-u^y_{lmn})+(v^z_{(l-1)(m-1)(n-1)}-u^z_{lmn})\\
&+(v^x_{l(m-1)(n-1)}-u^x_{lmn})-(v^y_{l(m-1)(n-1)}-u^y_{lmn})-(v^z_{l(m-1)(n-1)}-u^z_{lmn})\Big]\\
&+C_{\text{Cs-Cs}}\left(-2u^x_{lmn}+u^x_{(l-1)mn}+u^x_{(l+1)mn}\right),
\end{aligned}
$$

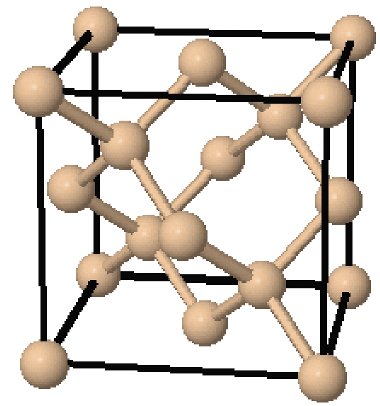
Two atoms per primitive unit cell





NaCl

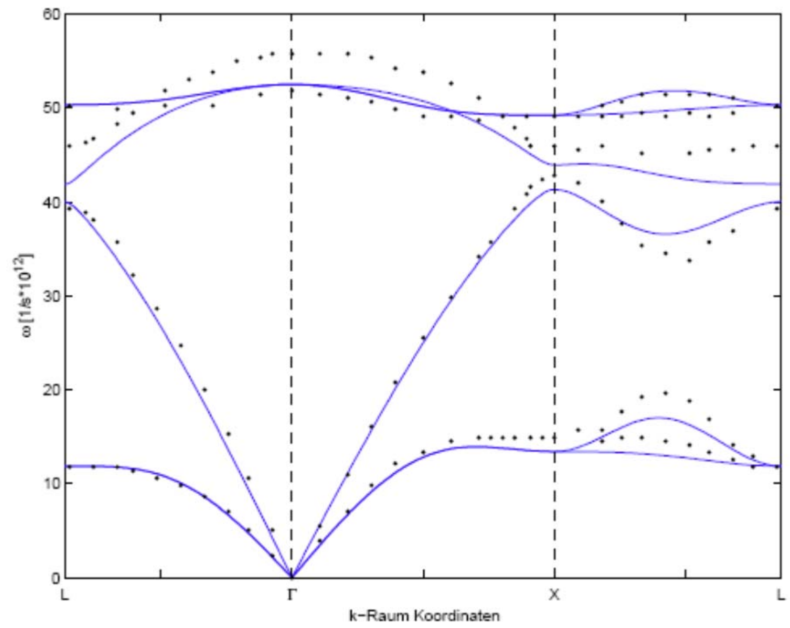


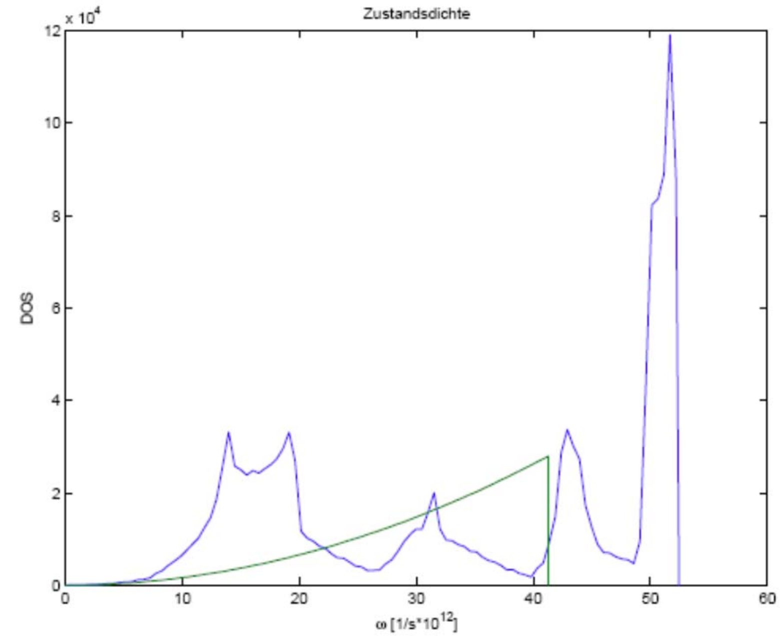


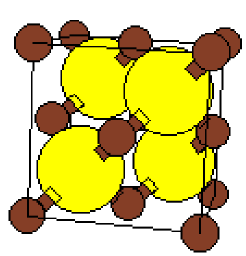
Si

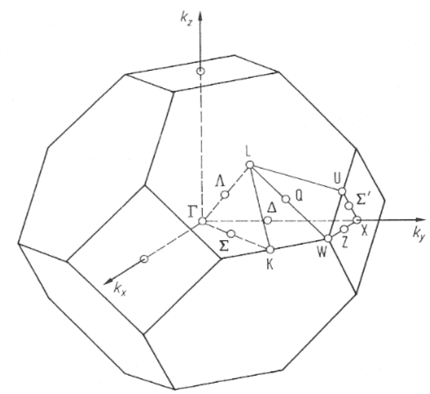
GaAs

Hannes Brandner

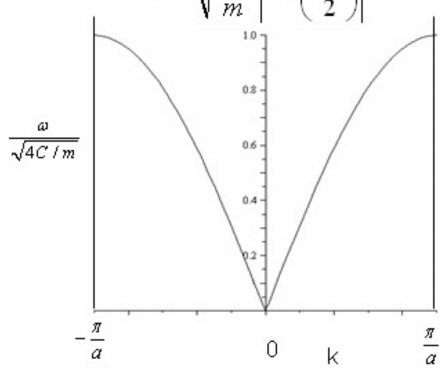
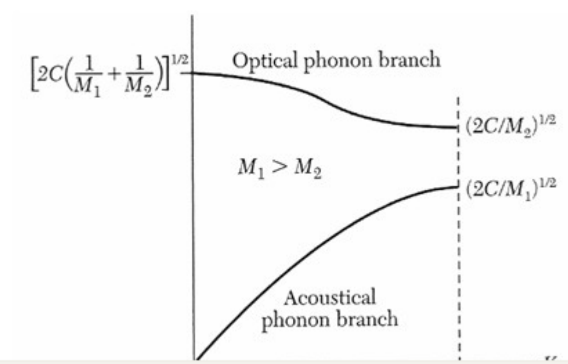








http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/phonontable.html

	Linear Chain $m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$	**Linear chain 2 masses** $M_1\frac{d^2u_s}{dt^2} = C(v_{s-1} - 2u_s + v_s)$ $M_2\frac{d^2v_s}{dt^2} = C(u_s - 2v_s + u_{s+1})$	**Linear chain 2 spring constants** $M\frac{d^2u_s}{dt^2} = C_1(v_{s-1} - 2u_s + v_s)$ $M\frac{d^2v_s}{dt^2} = C_2(u_s - 2v_s + u_{s+1})$	n
Eigenfunction solutions	$u_s = A_k e^{i(ksa-\omega t)}$	$u_s = ue^{i(ksa-\omega t)}$ $v_s = ve^{i(ksa-\omega t)}$	$u_s = ue^{i(ksa-\omega t)}$ $v_s = ve^{i(ksa-\omega t)}$	
Dispersion relation	$\omega = \sqrt{\frac{4C}{m}}\left\|\sin\left(\frac{ka}{2}\right)\right\|$ 	$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1M_2}}$ 		

Phonon quasiparticle lifetime

Phonons are the eigenstates of the linearized equations, not the full equations.

Phonons have a finite lifetime that can be calculated by Fermi's golden rule.

$$\Gamma_{i\rightarrow f} = \frac{2\pi}{\hbar}\left|\left\langle f \left| H_{ph-ph} \right| i \right\rangle\right|^2 \delta\left(E_f - E_i\right)$$

Occupation is determined by a master equation (not the Bose-Einstein function).

$$\begin{bmatrix} \frac{dP_0}{dt} \\ \frac{dP_1}{dt} \\ \vdots \\ \frac{dP_N}{dt} \end{bmatrix} = \begin{bmatrix} -\sum_{i\neq 0}\Gamma_{0\rightarrow i} & \Gamma_{1\rightarrow 0} & \cdots & \Gamma_{N\rightarrow 0} \\ \Gamma_{0\rightarrow 1} & -\sum_{i\neq 1}\Gamma_{1\rightarrow i} & \cdots & \Gamma_{N\rightarrow 1} \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma_{0\rightarrow N} & \Gamma_{1\rightarrow N} & \cdots & -\sum_{i\neq N}\Gamma_{N\rightarrow i} \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \\ \vdots \\ P_N \end{bmatrix}$$

Acoustic attenuation

The amplitude of a monocromatic sound wave decreases as the wave propagates through the crystal as the phonon quasiparticles decay into phonons with other frequencies and directions.