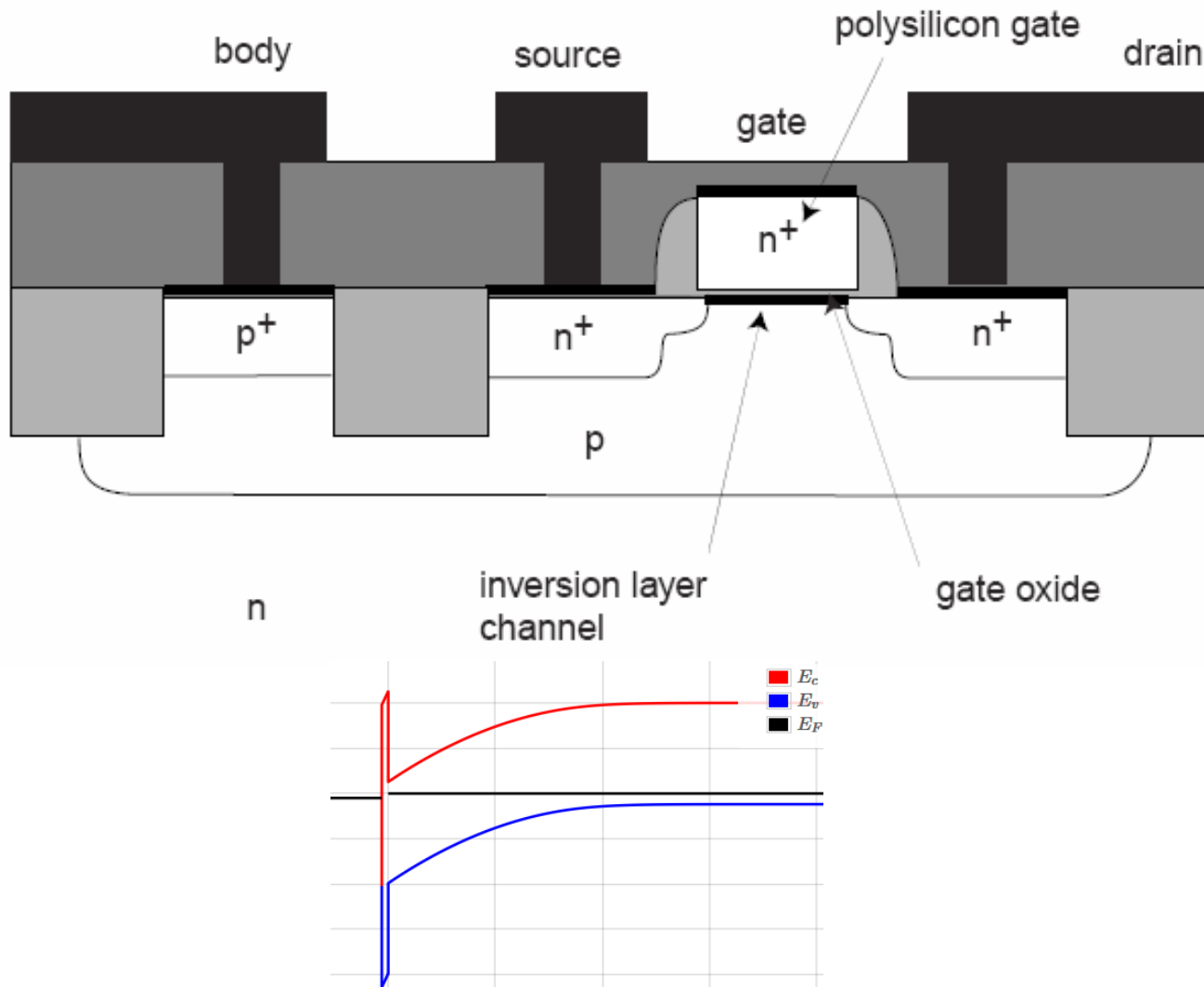


10. Semiconductors / Phonons

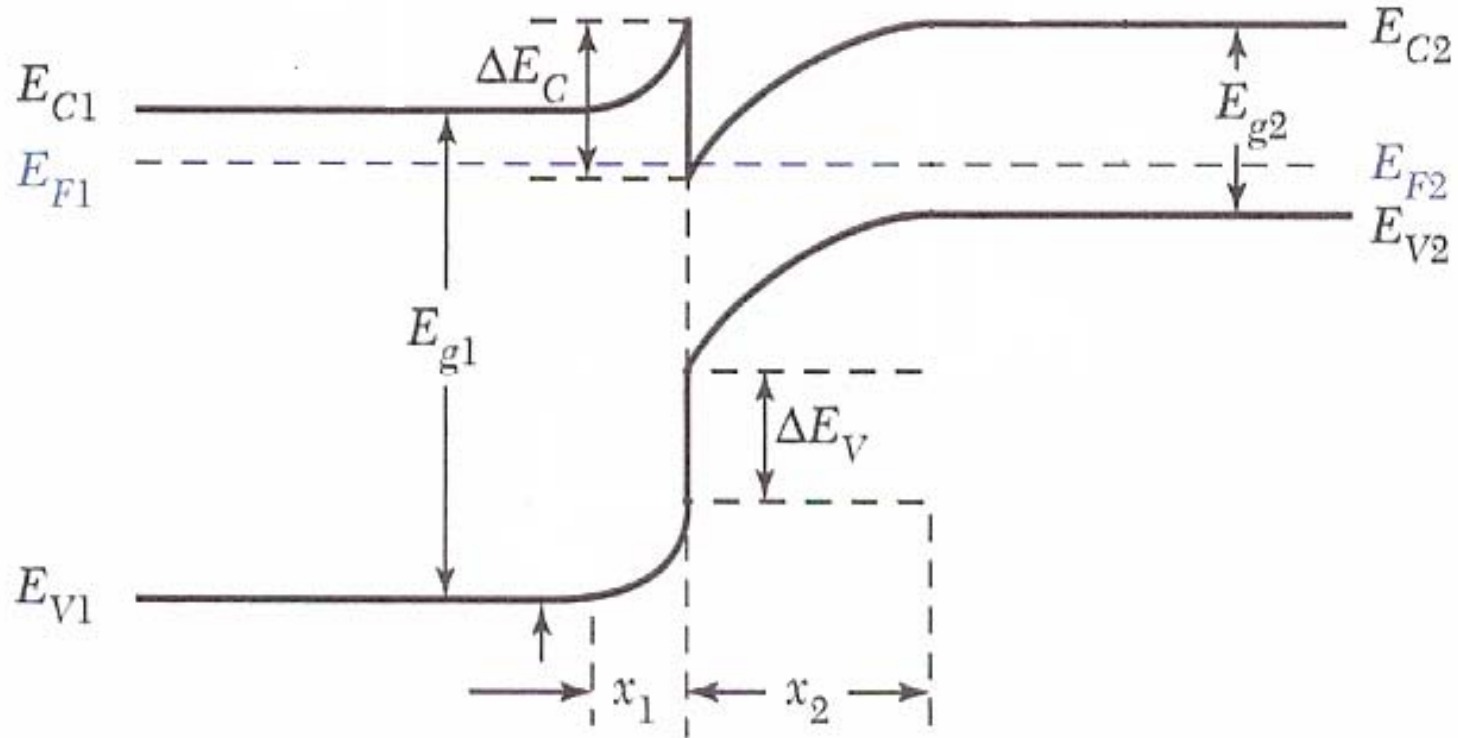
Nov 4, 2019

MOSFETs

Metal-oxide semiconductor field effect transistors

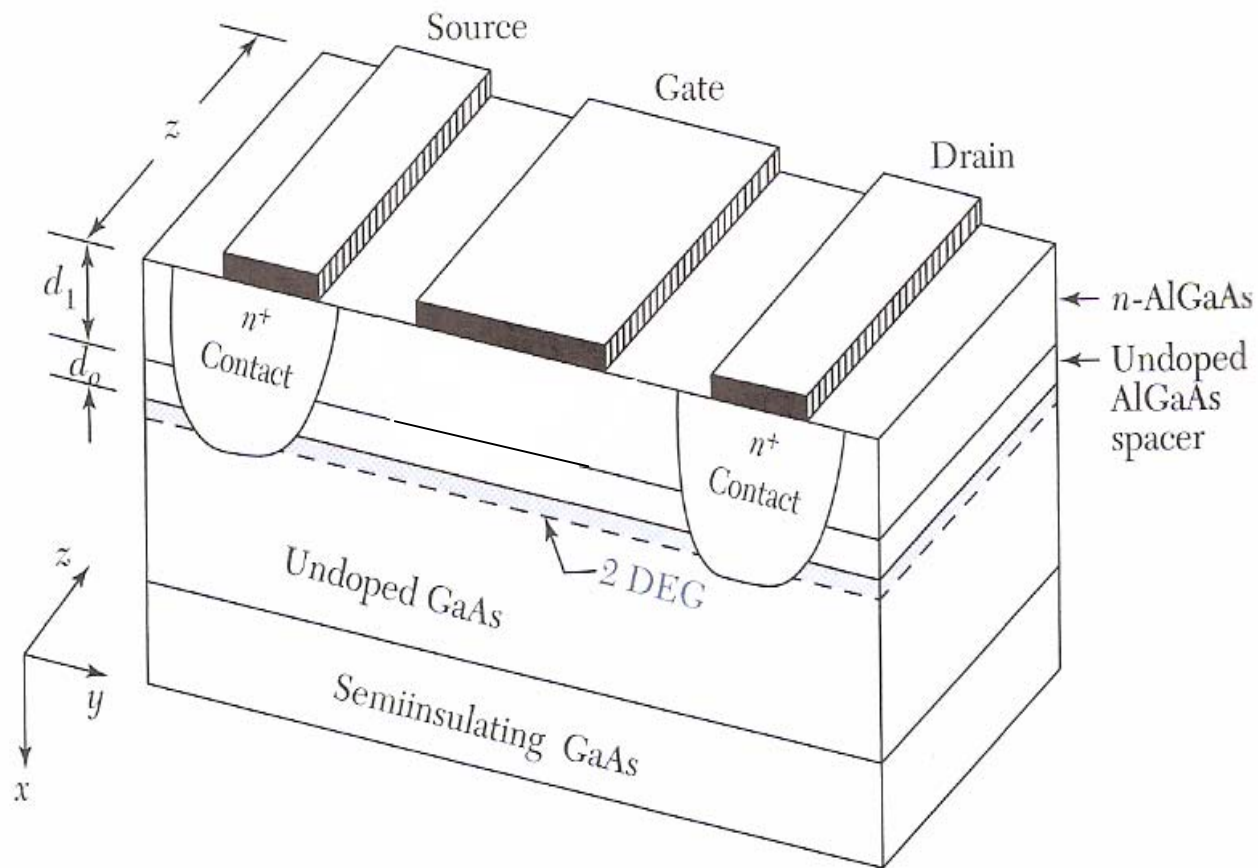


Heterojunctions



Quantum hall effect
Quantized conductance
HBTs
HEMTs

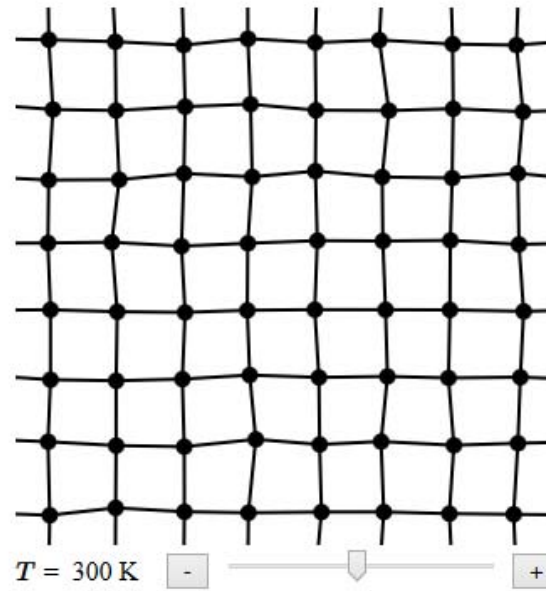
HEMT High electron mobility transistor

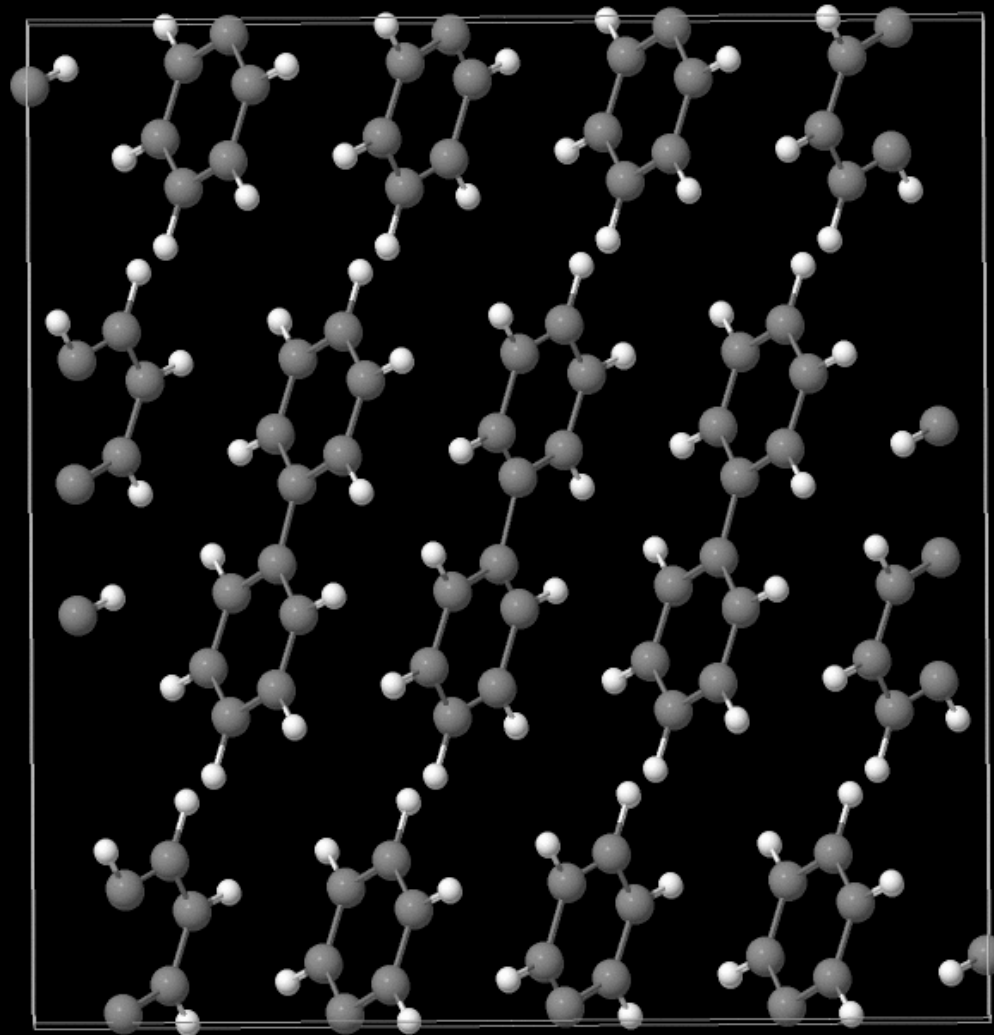


Phonons

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.

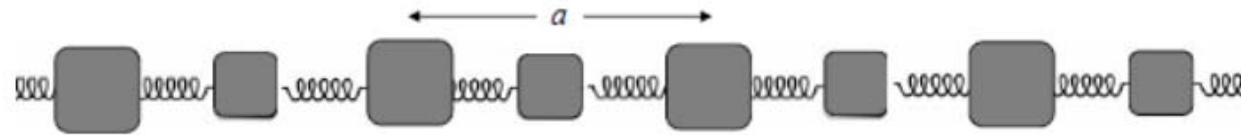




Natalia Bedoya

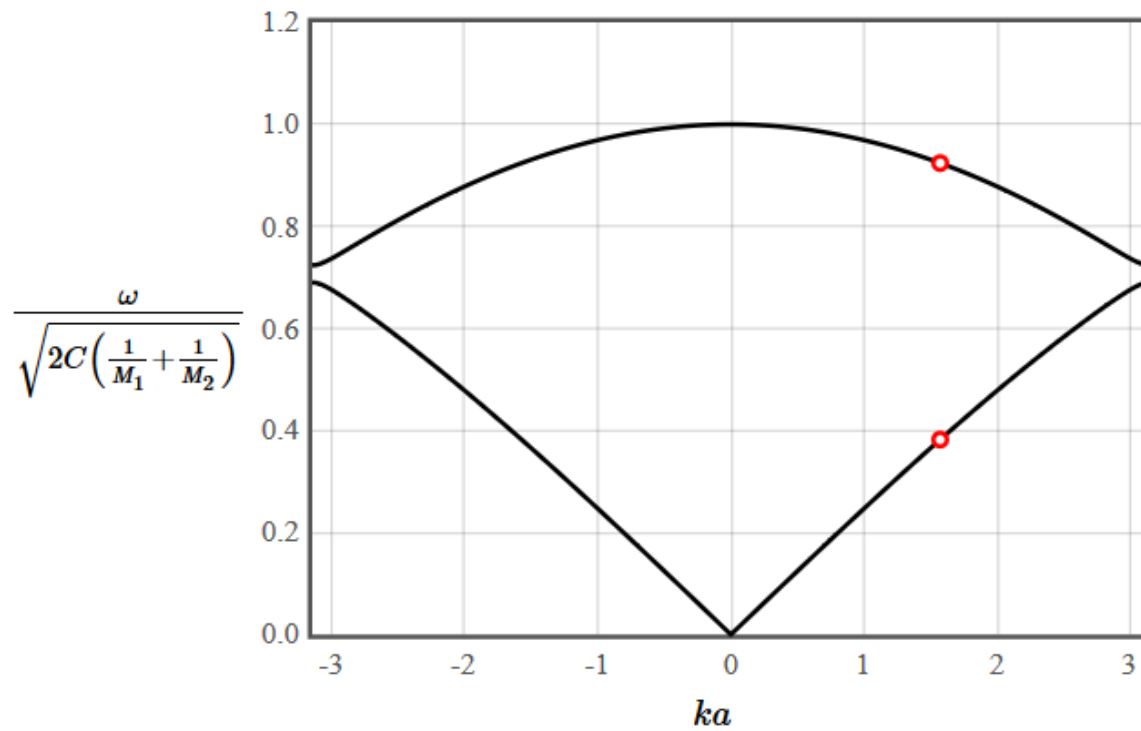
In a normal mode, all of the atoms oscillate at the same frequency.

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

$3N_{\text{atom}}$ 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

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

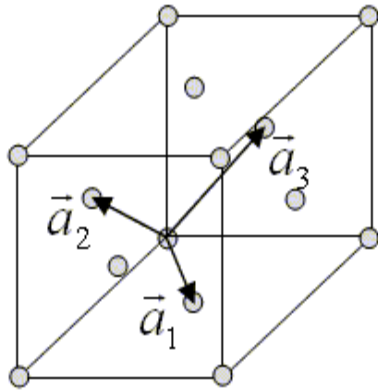
$$u_{lmn}^y = u_k^y \exp\left(i\left(l\vec{k} \cdot \vec{a}_1 + m\vec{k} \cdot \vec{a}_2 + n\vec{k} \cdot \vec{a}_3 - \omega t\right)\right)$$

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

These are eigenfunctions of T.

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

fcc



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

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

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

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

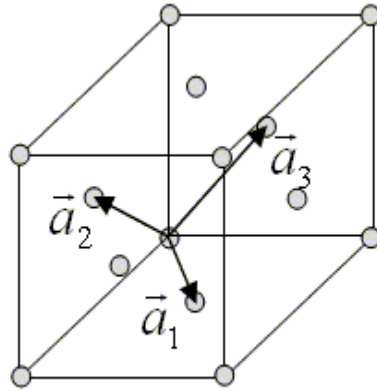
$$\vec{b}_2 = \frac{2\pi}{a} (\hat{k}_x - \hat{k}_y + \hat{k}_z)$$

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

$$\begin{aligned}
 m \frac{d^2 u_{lmn}^x}{dt^2} = & \frac{C}{2} \left[(u_{l+1mn}^x - u_{lmn}^x) + (u_{l-1mn}^x - u_{lmn}^x) + (u_{lm+1n}^x - u_{lmn}^x) + (u_{lm-1n}^x - u_{lmn}^x) \right. \\
 & + (u_{l+1mn-1}^x - u_{lmn}^x) + (u_{l-1mn+1}^x - u_{lmn}^x) + (u_{lm+1n-1}^x - u_{lmn}^x) + (u_{lm-1n+1}^x - u_{lmn}^x) \\
 & + (u_{l+1mn}^y - u_{lmn}^y) + (u_{l-1mn}^y - u_{lmn}^y) - (u_{lm+1n-1}^y - u_{lmn}^y) - (u_{lm-1n+1}^y - u_{lmn}^y) \\
 & \left. + (u_{lm+1n}^z - u_{lmn}^z) + (u_{lm-1n}^z - u_{lmn}^z) - (u_{l+1mn-1}^z - u_{lmn}^z) - (u_{l-1mn+1}^z - u_{lmn}^z) \right]
 \end{aligned}$$

and similar expressions for the y and z motion

fcc



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

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

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

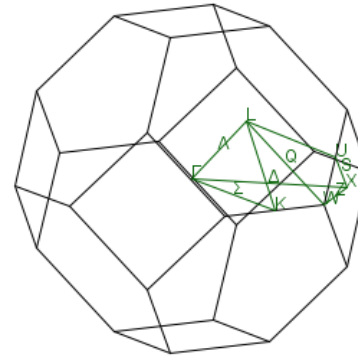
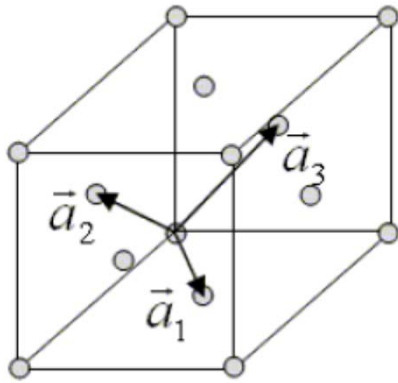
Substitute the eigenfunctions of T into Newton's laws.

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

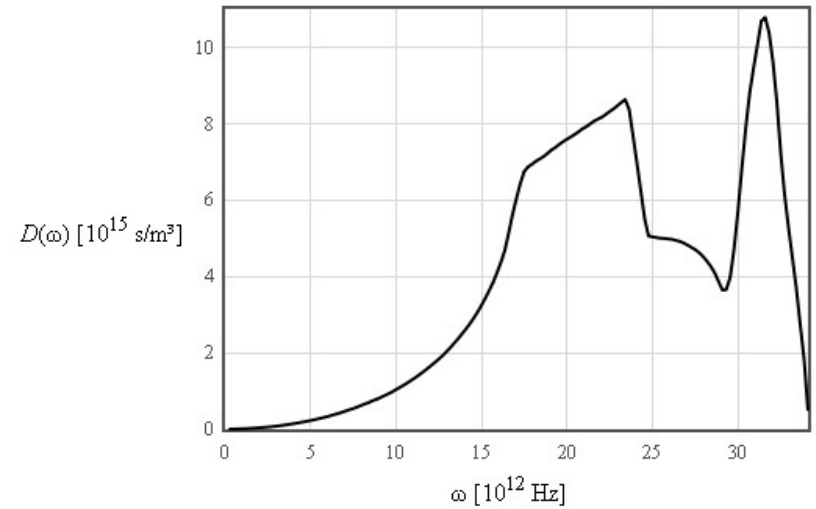
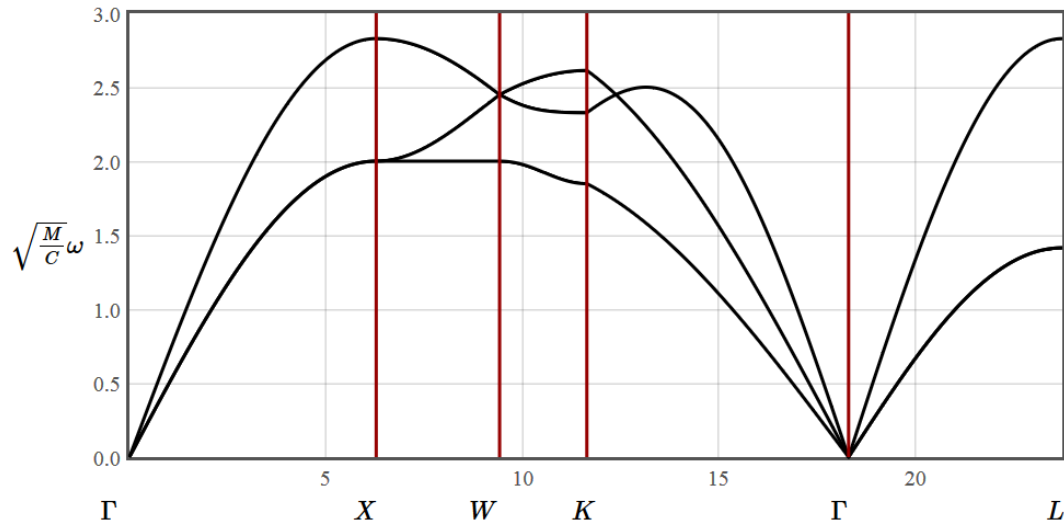
$$\begin{vmatrix} 4 - \cos\left(\frac{k_x a}{2} + \frac{k_y a}{2}\right) - \cos\left(\frac{k_x a}{2} + \frac{k_z a}{2}\right) - \cos\left(\frac{k_x a}{2} - \frac{k_y a}{2}\right) - \cos\left(\frac{k_x a}{2} - \frac{k_z a}{2}\right) - \frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_x a}{2} + \frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_y a}{2}\right) & -\cos\left(\frac{k_x a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_z a}{2}\right) \\ -\cos\left(\frac{k_x a}{2} + \frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_y a}{2}\right) & 4 - \cos\left(\frac{k_y a}{2} + \frac{k_z a}{2}\right) - \cos\left(\frac{k_y a}{2} + \frac{k_x a}{2}\right) - \cos\left(\frac{k_y a}{2} - \frac{k_x a}{2}\right) - \cos\left(\frac{k_y a}{2} - \frac{k_z a}{2}\right) - \frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_y a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2} - \frac{k_z a}{2}\right) \\ -\cos\left(\frac{k_x a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_z a}{2}\right) & -\cos\left(\frac{k_y a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2} - \frac{k_z a}{2}\right) & 4 - \cos\left(\frac{k_z a}{2} + \frac{k_x a}{2}\right) - \cos\left(\frac{k_z a}{2} + \frac{k_y a}{2}\right) - \cos\left(\frac{k_z a}{2} - \frac{k_x a}{2}\right) - \cos\left(\frac{k_z a}{2} - \frac{k_y a}{2}\right) - \frac{m\omega^2}{\sqrt{2}C} \end{vmatrix} = 0$$

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

fcc phonons



$3N$ degrees of freedom



Phonon dispersion Au

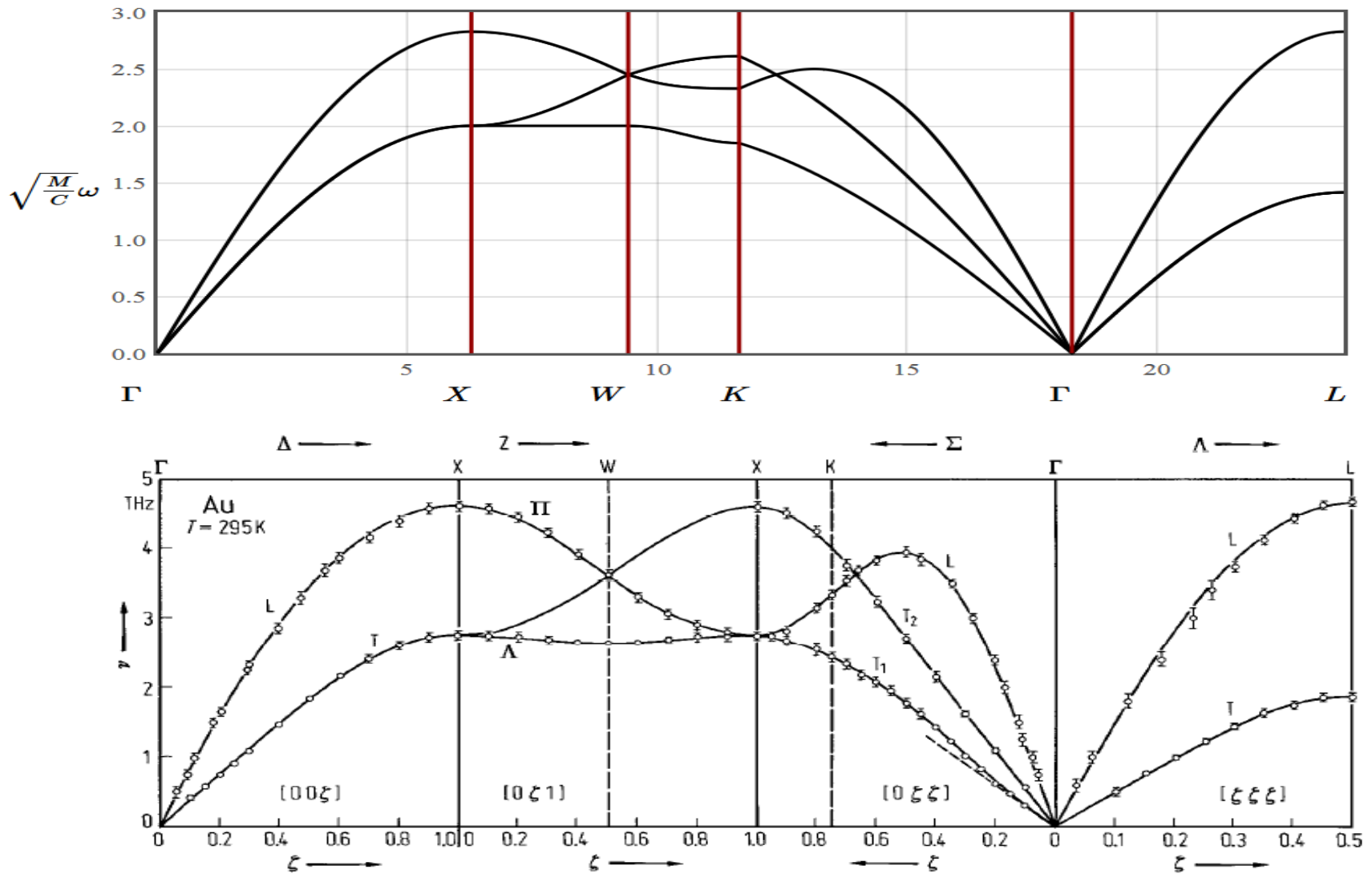
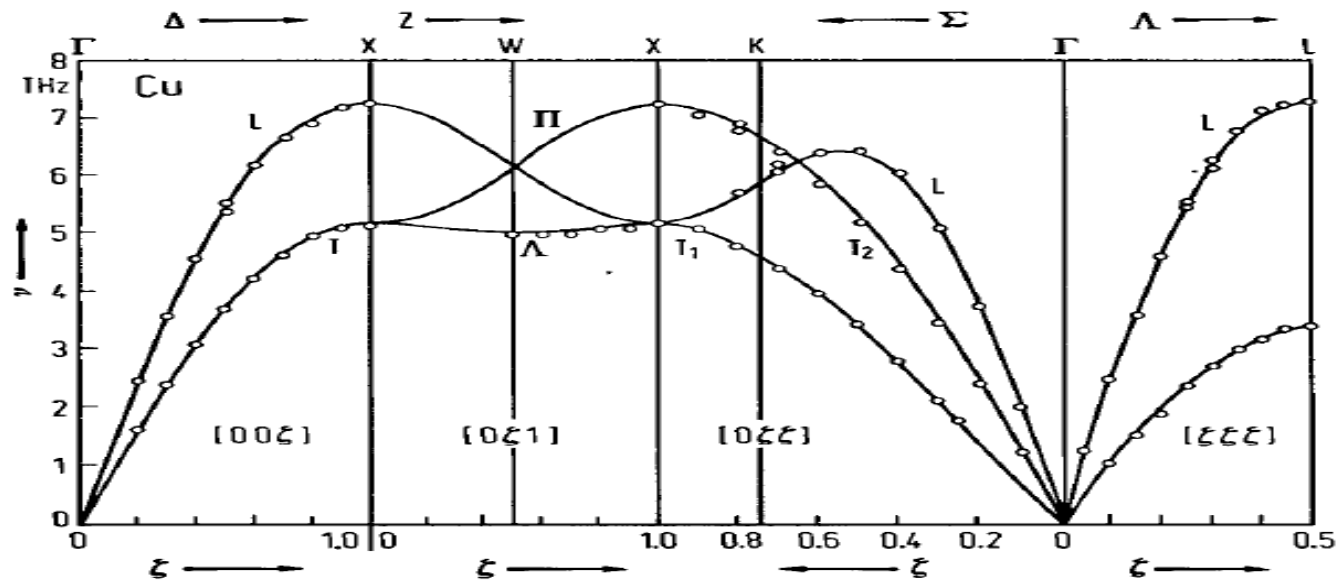
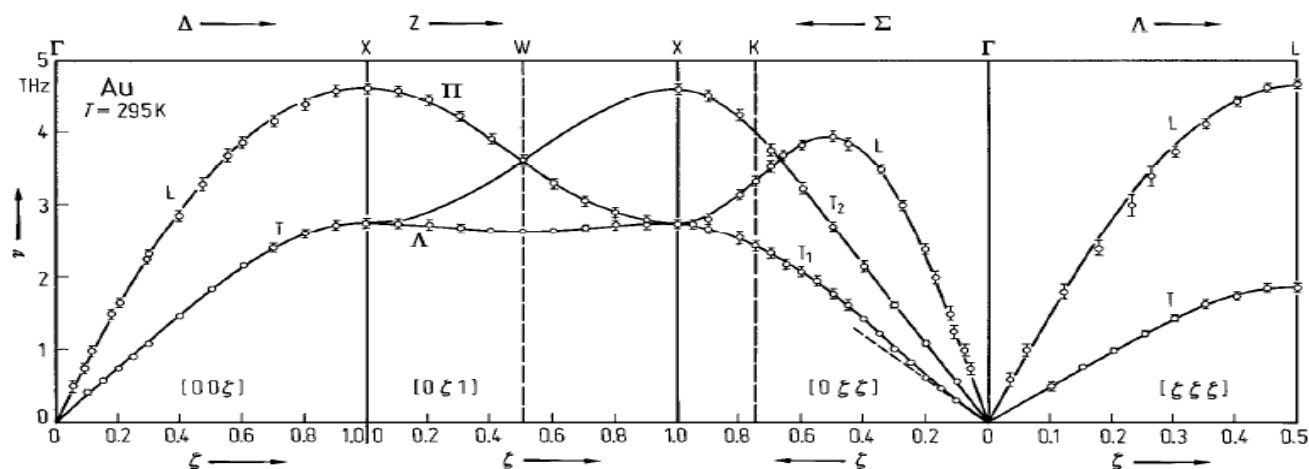


Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the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

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



Cu



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 $[0\xi\xi] T_1$ branch.

fcc phonons

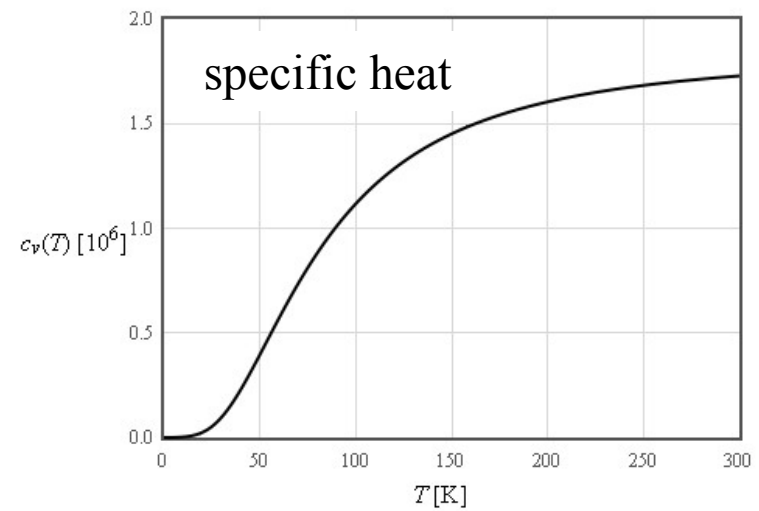
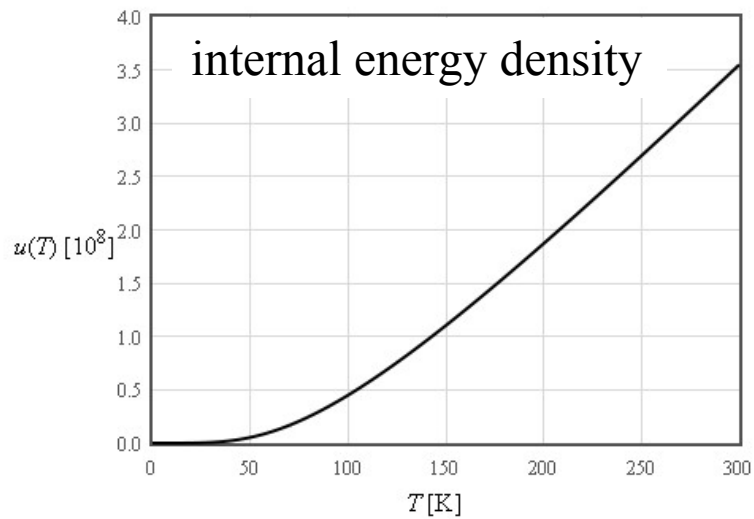
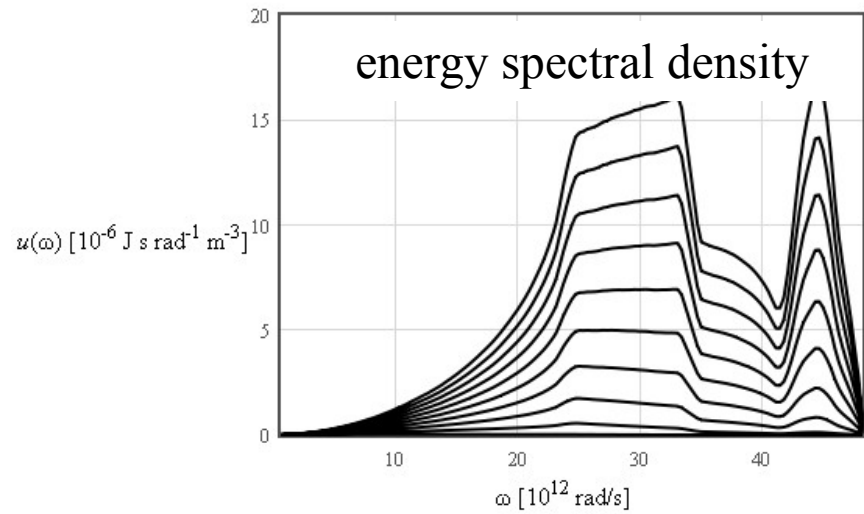
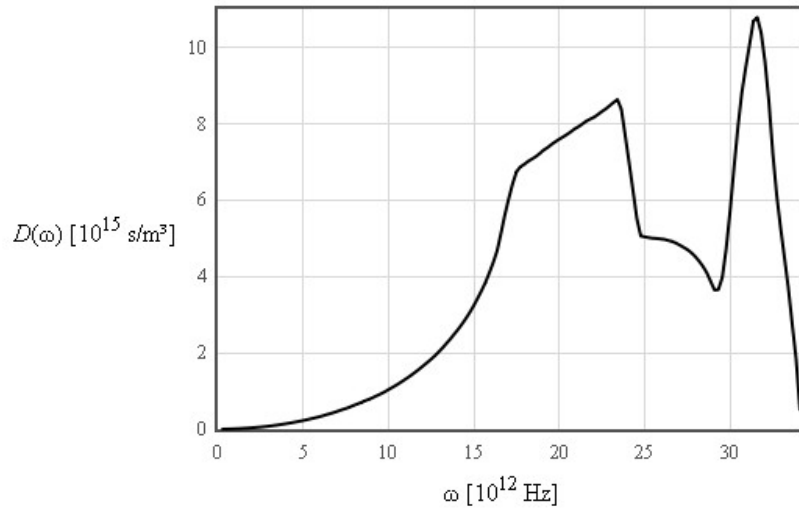
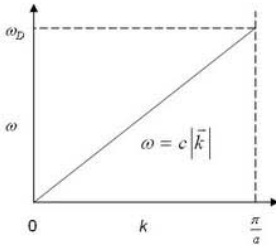
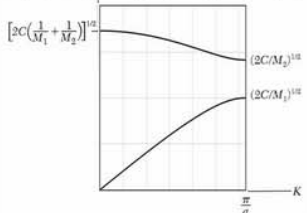
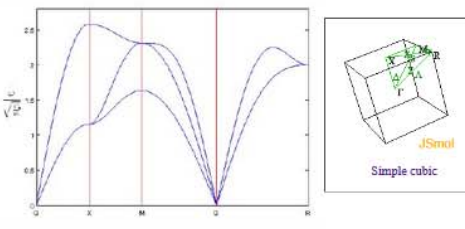
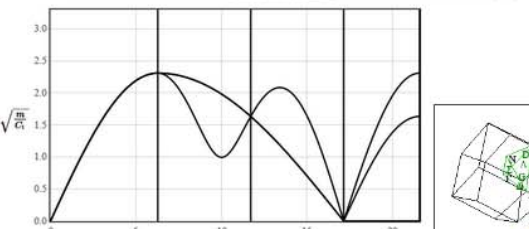
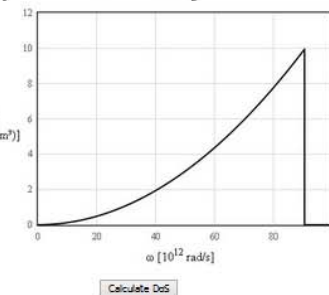
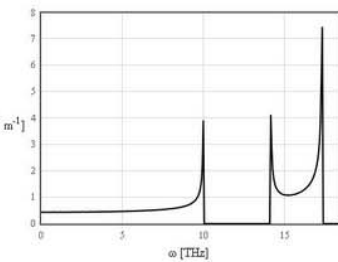
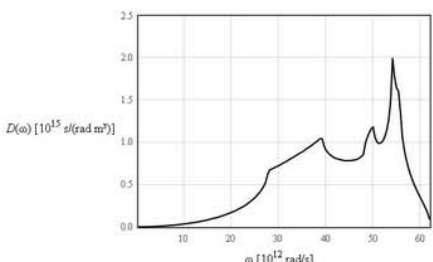
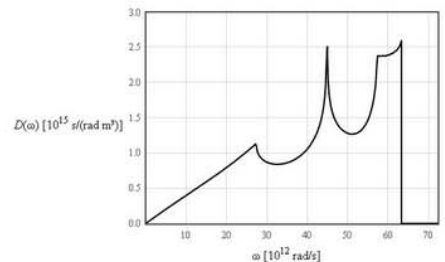
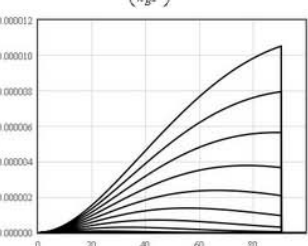
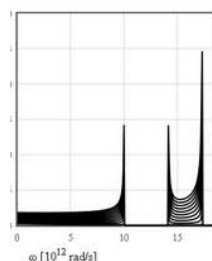
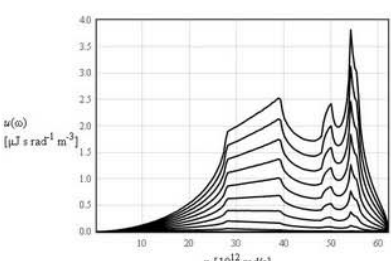
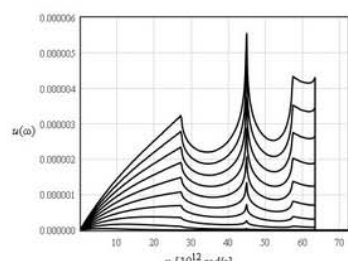


Table summarizing the thermodynamic properties of phonons

 <p>$\omega = c \vec{k}$</p>	$\omega^2 = C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4}{M_1 M_2}}$  <p>Calculate $\omega(k)$</p>	 <p>Simple cubic</p>	$\begin{aligned} & \frac{1}{2} (u_{i-1,m-1,n-1}^2 - u_{i,m,n}^2) + \frac{1}{2} (u_{i-1,m-1,n-1}^2 - u_{i,m,n}^2) \\ & \frac{1}{2} (u_{i-1,m-1,n-1}^2 - u_{i,m,n}^2) + \frac{1}{2} (u_{i+1,m+1,n+1}^2 - u_{i,m,n}^2) \\ & \frac{1}{2} (u_{i+1,m+1,n+1}^2 - u_{i,m,n}^2) + \frac{1}{2} (u_{i+1,m+1,n+1}^2 - u_{i,m,n}^2) \\ & + \left\{ \begin{array}{l} C_{11}(u_{i+1,m+1,n}^2 - 2u_{i,m,n}^2 + u_{i-1,m-1,n}^2) \\ C_{44}(u_{i+1,m,n+1}^2 - 2u_{i,m,n}^2 + u_{i-1,m,n-1}^2) \\ C_{44}(u_{i,m+1,n+1}^2 - 2u_{i,m,n}^2 + u_{i,m-1,n-1}^2) \end{array} \right\} \\ & \text{nearest-neighbour} \end{aligned}$  <p>Body centered</p> <p>Calculate $\omega(k)$</p>
$D(k) = \frac{3k^2}{2\pi^2}$ $v(\omega) = \begin{cases} \frac{3\omega^2}{2\pi^2 c^3} & \text{for } \omega < \omega_D = (6n\pi^2 c^3)^{1/3} \\ 0 & \text{for } \omega > \omega_D \end{cases} \quad [\text{s rad}^{-1} \text{m}^{-3}]$  <p>Calculate DoS</p>	$D(k) = \frac{1}{\pi}$  <p>Calculate DoS</p>	$D(k) = \frac{3k^2}{2\pi^2}$  <p>Calculate DoS</p>	$D(k) = \frac{3k^2}{2\pi^2}$  <p>Calculate DoS</p>
$\mu(\omega) = \frac{3\omega^2}{2\pi^2 c^3} \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} \quad [\text{J s m}^{-3}]$ 			

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

- **Phonons**

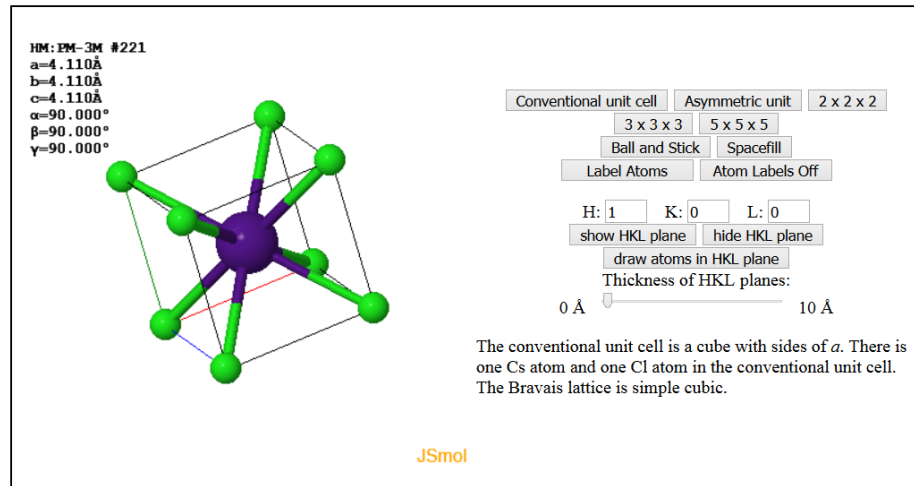
- Normal modes and phonons

- Using complex numbers to represent sinusoidal oscillations
 - Linear chain
 - Linear chain with two different masses
 - fcc with linear springs to nearest neighbors
 - bcc with linear springs to nearest neighbors
 - CsCl

- Thermodynamic properties of non-interacting bosons

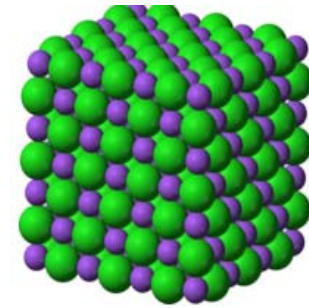
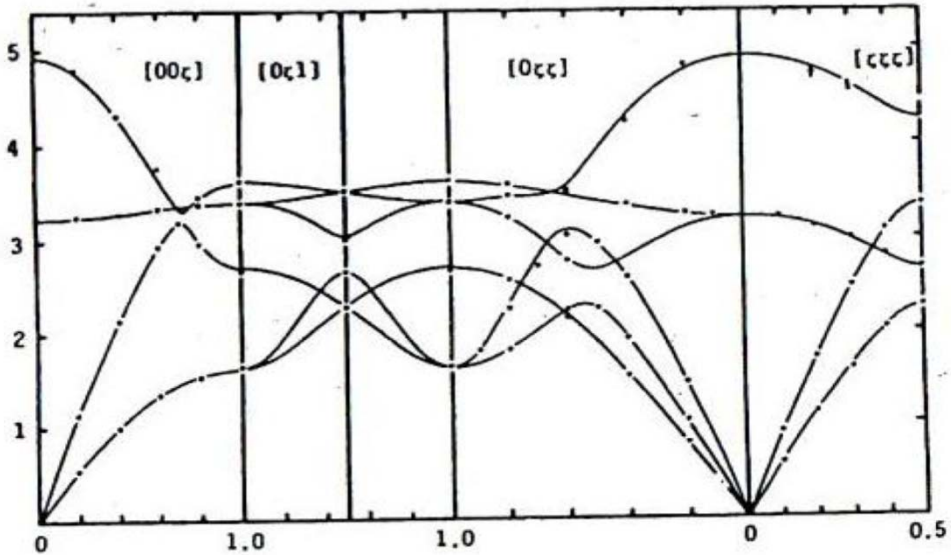
- Density of states
 - simple cubic, bcc, fcc
 - Ag-fcc, Al-fcc, AlN, Au-fcc, Fe-bcc, GaN, Mg-hcp, Mo-bcc, Si-diamond, α -Sn, β -Sn, Ta-bcc, Tb-hcp, Ti-hcp, W-bcc, ZnO (rocksalt), ZnO (zincblende), ZnO (wurtzite), Zr-hcp
 - Energy spectral density $u(\omega, T)$
 - Internal energy density $u(T)$
 - Specific heat $c_v(T)$
 - Helmholtz free energy density $f(T)$
 - Entropy density $s(T)$
 - Table summarizing the thermodynamic properties of phonons

Phonon dispersion of CsCl

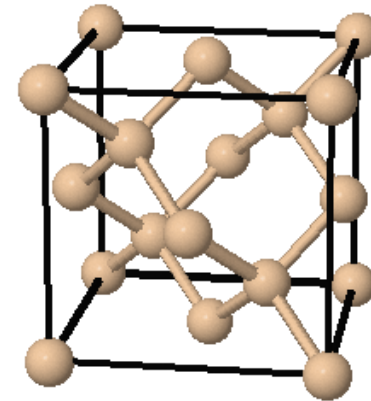
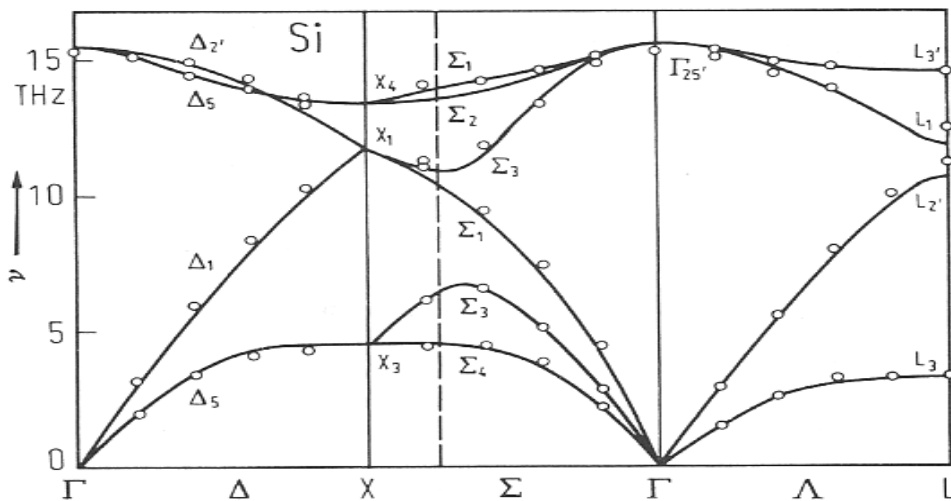


$$\begin{aligned}
 M_{\text{Cs}} \frac{d^2 u_{lmn}^x}{dt^2} = & \frac{C_{\text{Cs-Cl}}}{3} \left[+ (v_{lmn}^x - u_{lmn}^x) + (v_{lmn}^y - u_{lmn}^y) + (v_{lmn}^z - u_{lmn}^z) \right. \\
 & + (v_{(l-1)mn}^x - u_{lmn}^x) - (v_{(l-1)mn}^y - u_{lmn}^y) - (v_{(l-1)mn}^z - u_{lmn}^z) \\
 & + (v_{(l-1)(m-1)n}^x - u_{lmn}^x) + (v_{(l-1)(m-1)n}^y - u_{lmn}^y) - (v_{(l-1)(m-1)n}^z - u_{lmn}^z) \\
 & + (v_{l(m-1)n}^x - u_{lmn}^x) - (v_{l(m-1)n}^y - u_{lmn}^y) + (v_{l(m-1)n}^z - u_{lmn}^z) \\
 & + (v_{lm(n-1)}^x - u_{lmn}^x) + (v_{lm(n-1)}^y - u_{lmn}^y) - (v_{lm(n-1)}^z - u_{lmn}^z) \\
 & + (v_{(l-1)m(n-1)}^x - u_{lmn}^x) - (v_{(l-1)m(n-1)}^y - u_{lmn}^y) + (v_{(l-1)m(n-1)}^z - u_{lmn}^z) \\
 & + (v_{(l-1)(m-1)(n-1)}^x - u_{lmn}^x) + (v_{(l-1)(m-1)(n-1)}^y - u_{lmn}^y) + (v_{(l-1)(m-1)(n-1)}^z - u_{lmn}^z) \\
 & \left. + (v_{l(m-1)(n-1)}^x - u_{lmn}^x) - (v_{l(m-1)(n-1)}^y - u_{lmn}^y) - (v_{l(m-1)(n-1)}^z - u_{lmn}^z) \right] \\
 & + C_{\text{Cs-Cs}} \left(-2u_{lmn}^x + u_{(l-1)mn}^x + u_{(l+1)mn}^x \right),
 \end{aligned}$$

Two atoms per primitive unit cell



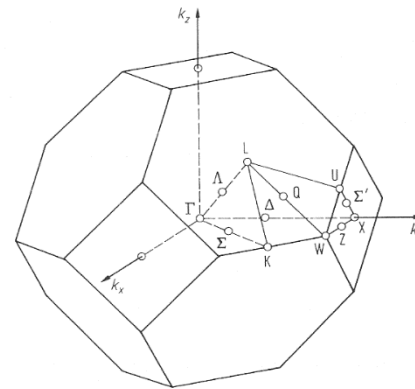
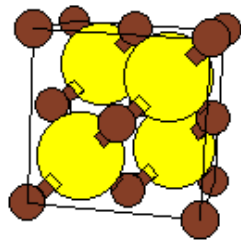
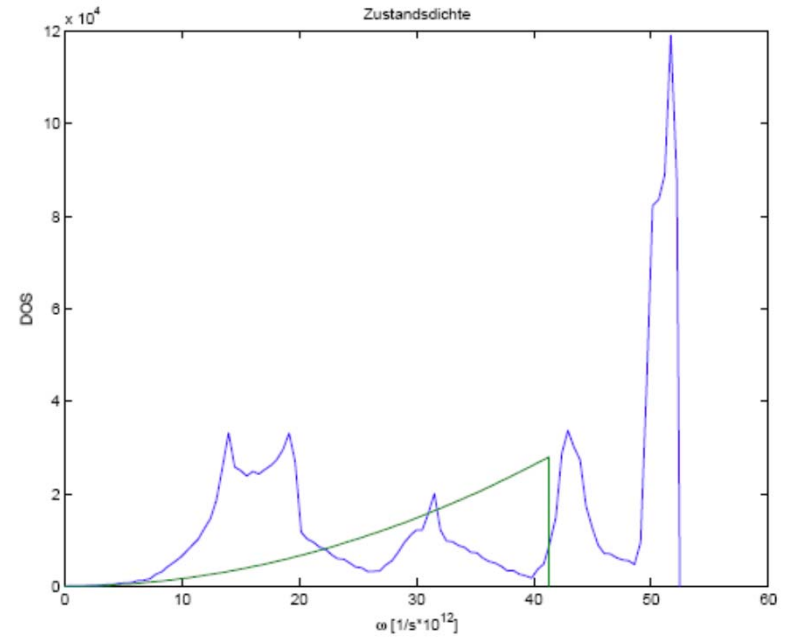
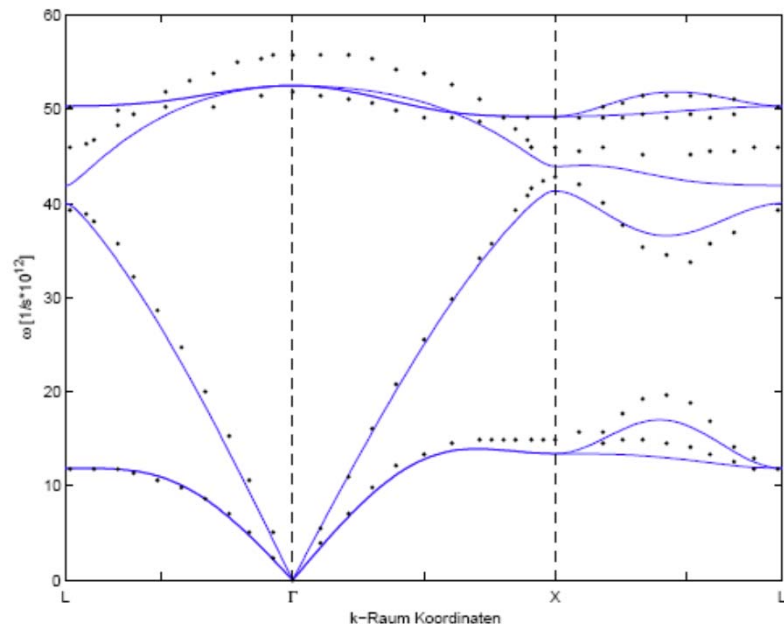
NaCl



Si

GaAs

Hannes Brandner



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.

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

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 monochromatic sound wave decreases as the wave propagates through the crystal as the phonon quasiparticles decay into phonons with other frequencies and directions.

Welcome to phonopy

Phonopy is an open source package for phonon calculations at harmonic and quasi-harmonic levels.

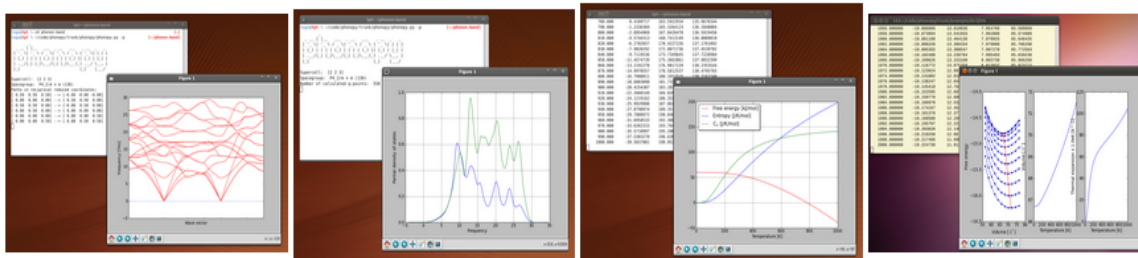
Phono3py is another open source package for phonon-phonon interaction and lattice thermal conductivity calculations. See the documentation at <http://atztoigo.github.io/phono3py/>

Phonon database: A collection of first principles phonon calculations is available as open data at <http://phonondb.mtl.kyoto-u.ac.jp/>, where the raw data of phonopy & VASP results are downloaded.

The following features of phonopy are highlighted:

- Phonon band structure, phonon DOS and partial-DOS
- Phonon thermal properties: Free energy, heat capacity (Cv), and entropy
- Phonon group velocity
- Thermal ellipsoids / Mean square displacements
- Irreducible representations of normal modes
- Dynamic structure factor for INS and IXS
- Non-analytical-term correction: LO-TO splitting (Born effective charges and dielectric constant are required.)
- Mode Grüneisen parameters
- Quasi-harmonic approximation: Thermal expansion, heat capacity at constant pressure (Cp)
- Interfaces to calculators: VASP, VASP DFPT, ABINIT, Quantu ESPRESSO, SIESTA, Elk, FHI-aims, WIEN2k, CRYSTAL, LAMMPS (external)
- Phonopy API for Python

A presentation in pdf for introduction to phonopy is downloaded *****here*****.



Student projects

Calculate the phonon dispersion and/or phonon density of states for some crystal.

Explain how to use a band structure program like Quantum Espresso or VASP to calculate the phonon dispersion.

Explain how to use Phonopy to plot phonon dispersion, densities of states, and to animate phonon modes.