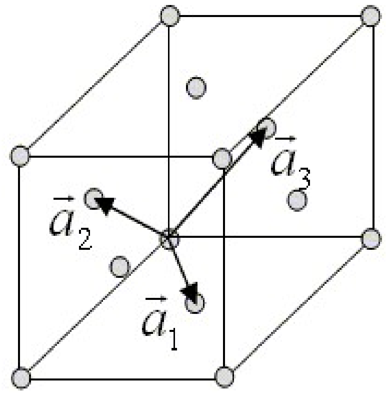
Phonon bandstructures

fcc



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

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

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

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

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

Normal modes are eigenfunctions of T

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

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

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

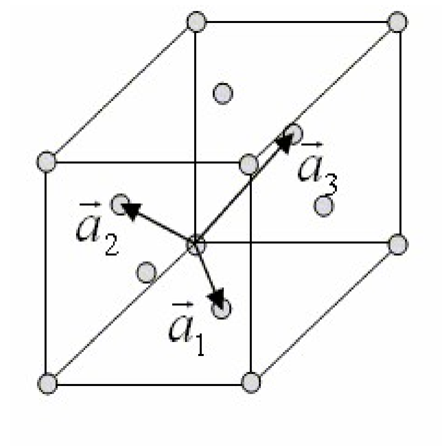
These are eigenfunctions of T.

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

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

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

fcc



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

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

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

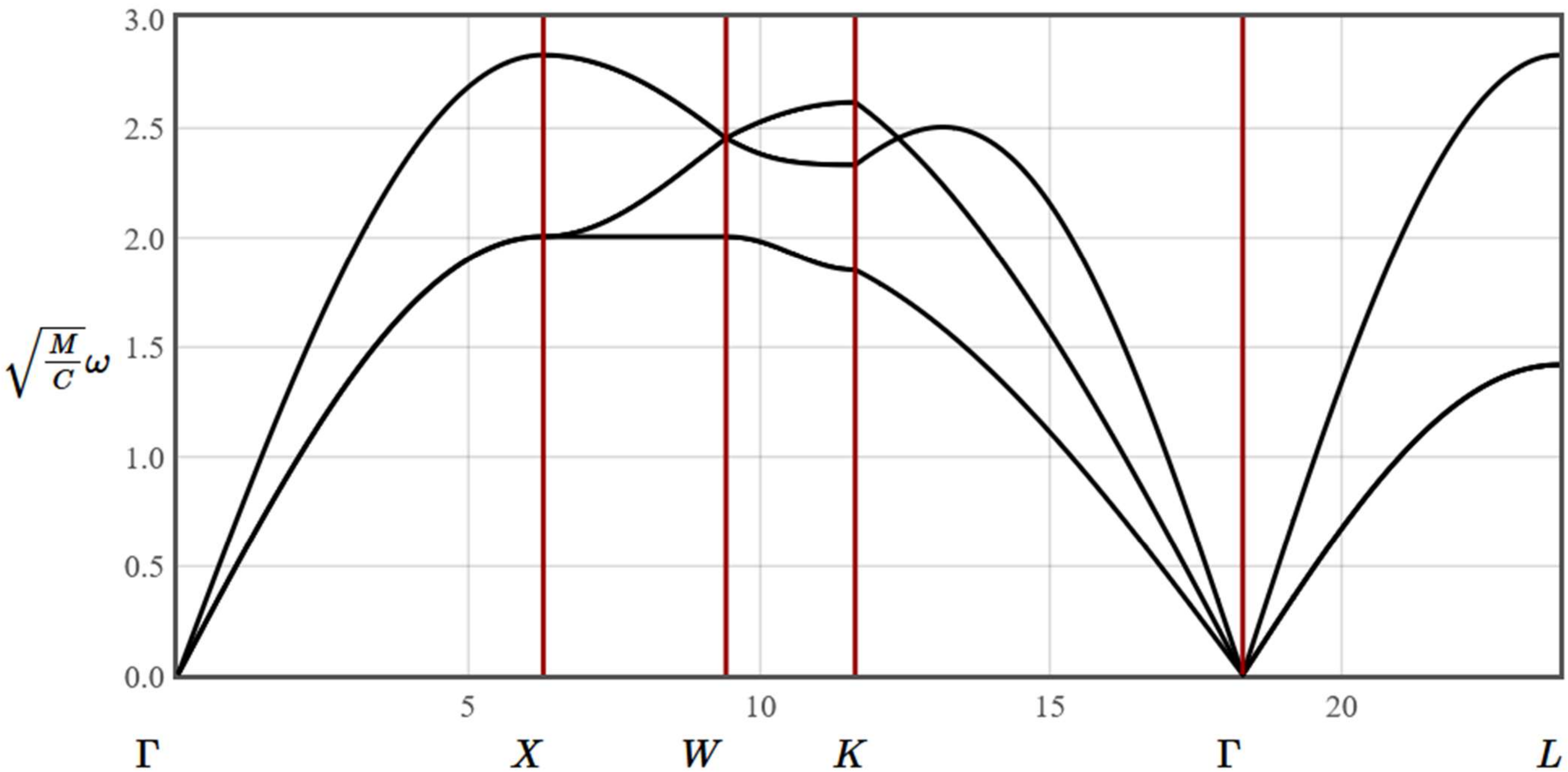
Substitute the eigenfunctions of *T* into Newton's laws.

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

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

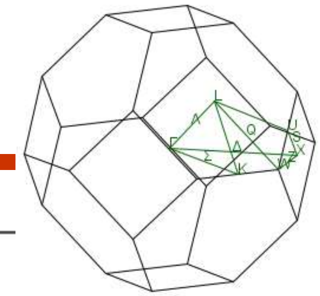
http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/fcc/fcc.html

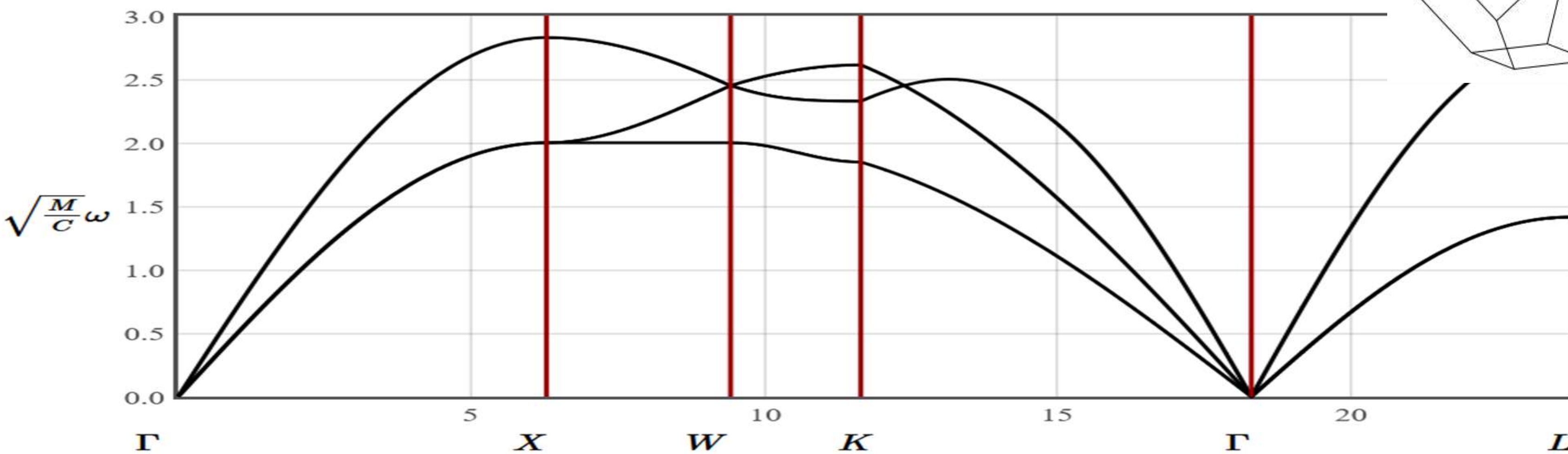
For every *k* there are 3 solutions for ω.



Phonon dispersion Au

From Springer Materials: Landholt Boernstein Database





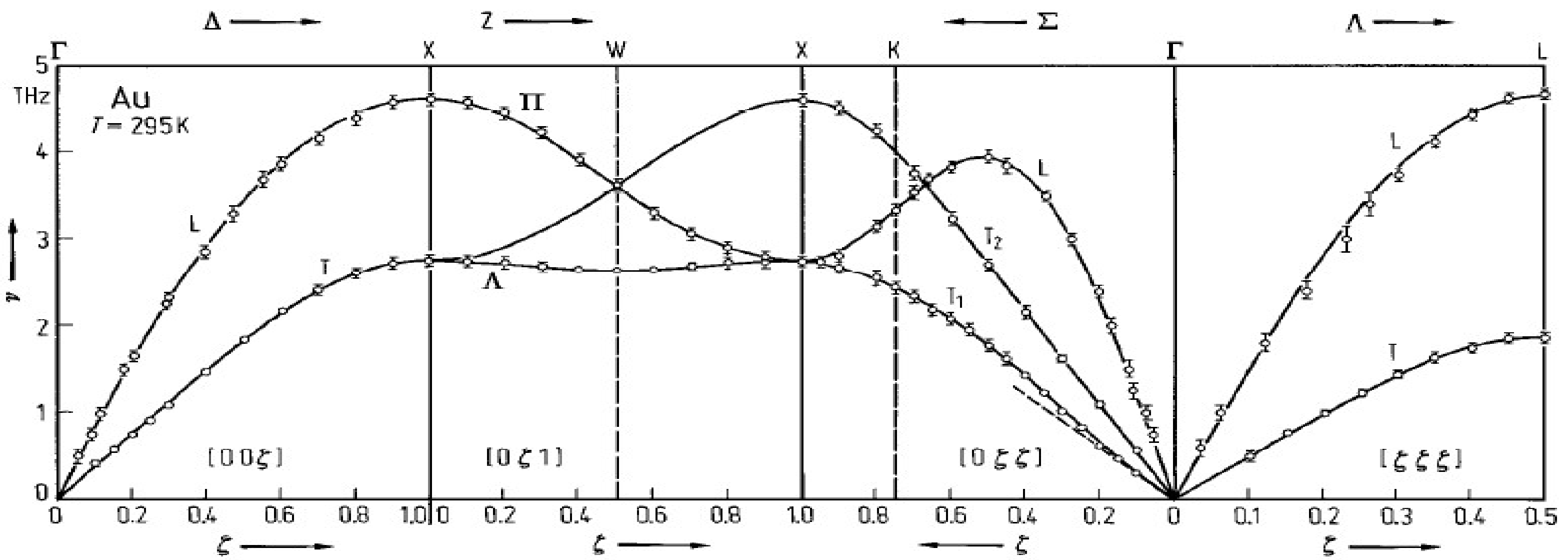
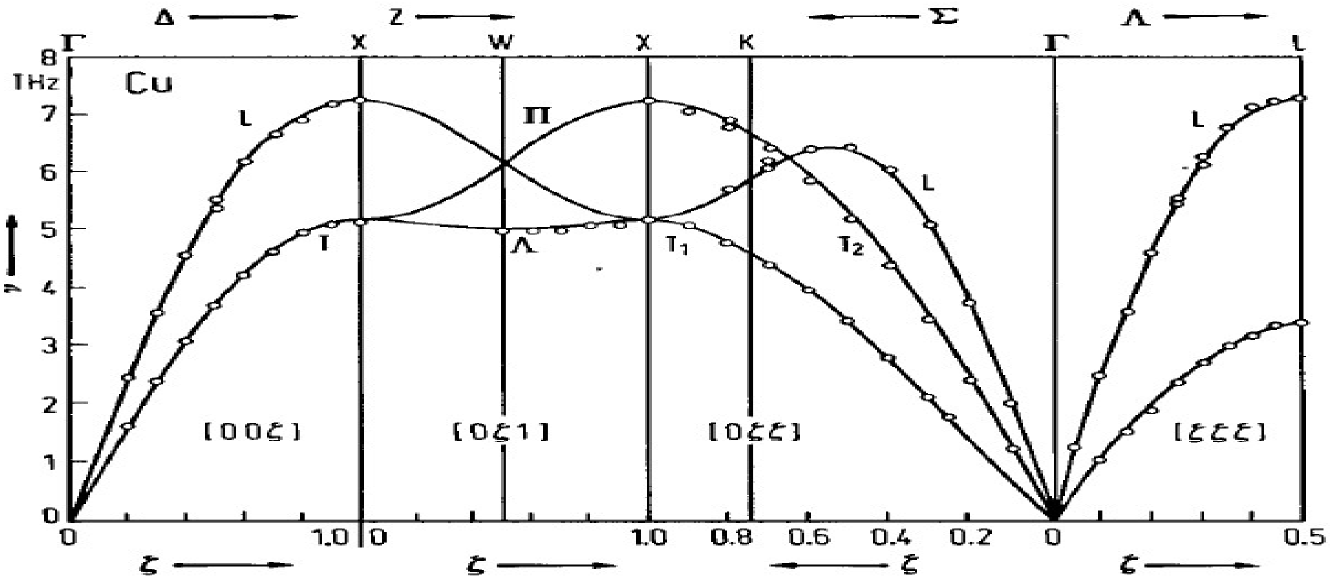
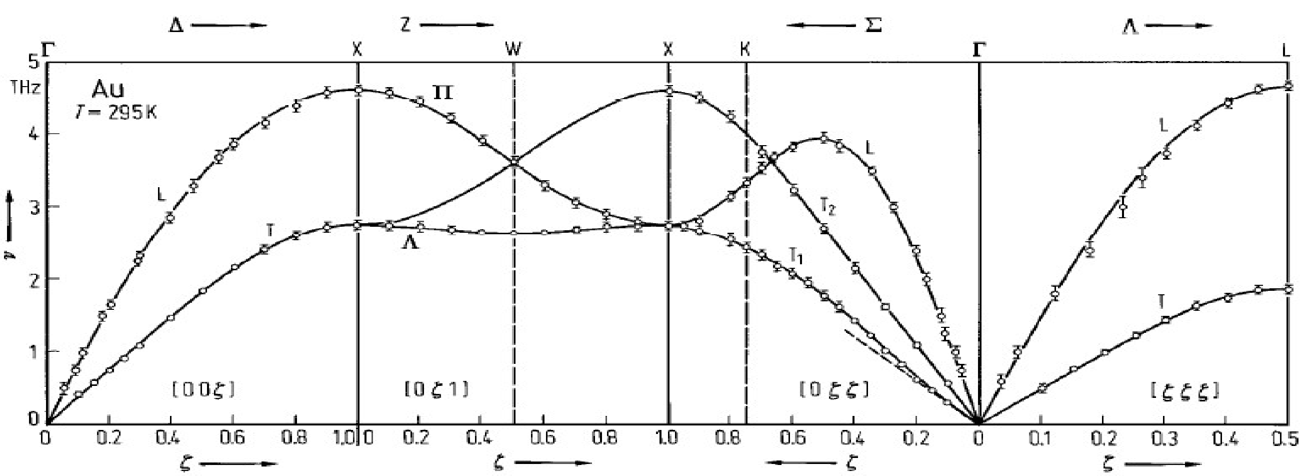


Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M 1) and the fifth neighbour axially symmetric model (M 2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the [0ζζ] T_1 branch.

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



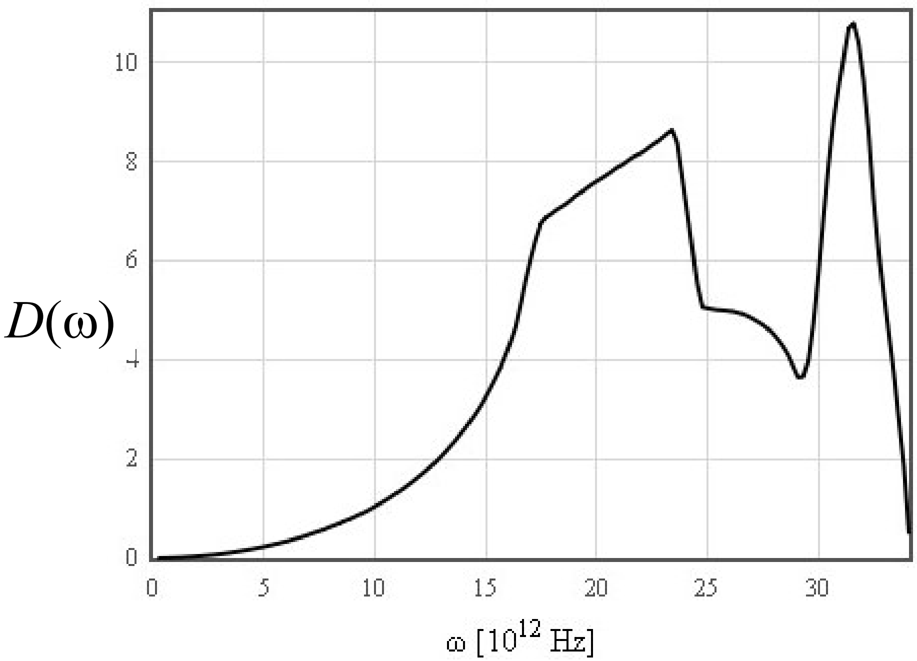
Cu



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 (M 2) 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.

Phonon DOS fcc



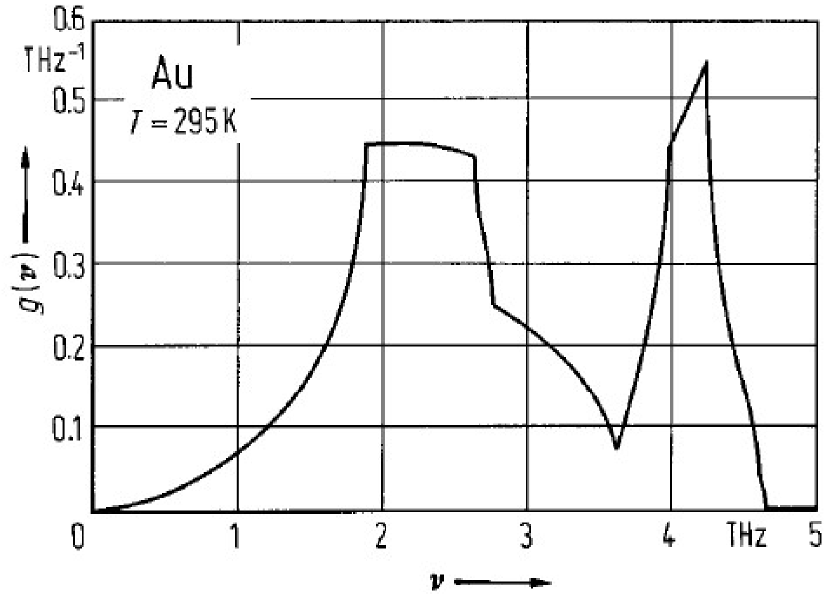
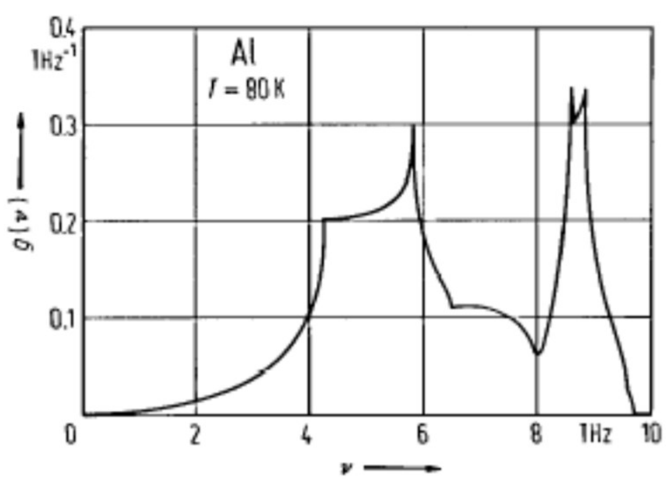
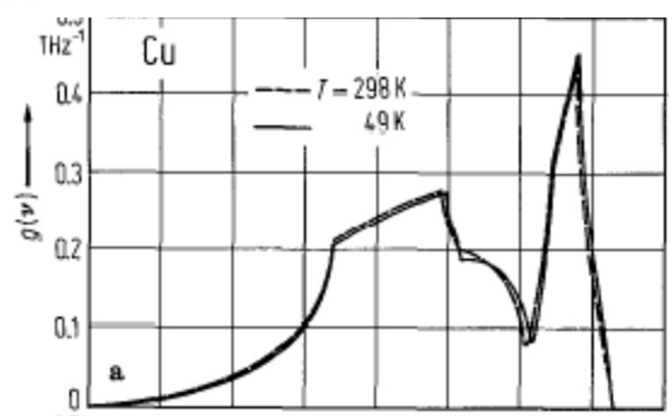


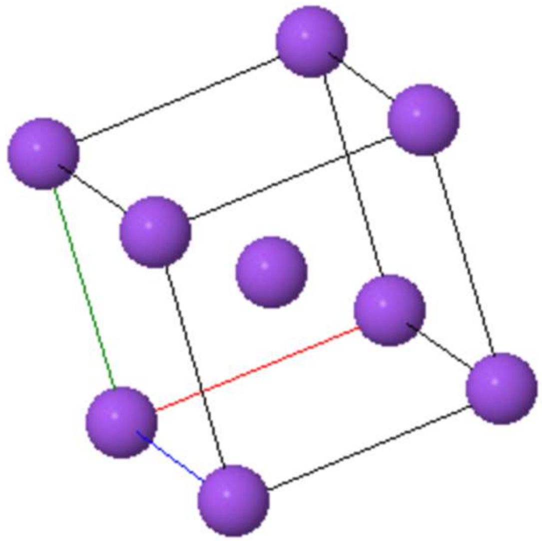
Fig. 2. Au. Frequency distribution calculated from the fourth neighbour general force constant model (M1) of Table 3 Au.

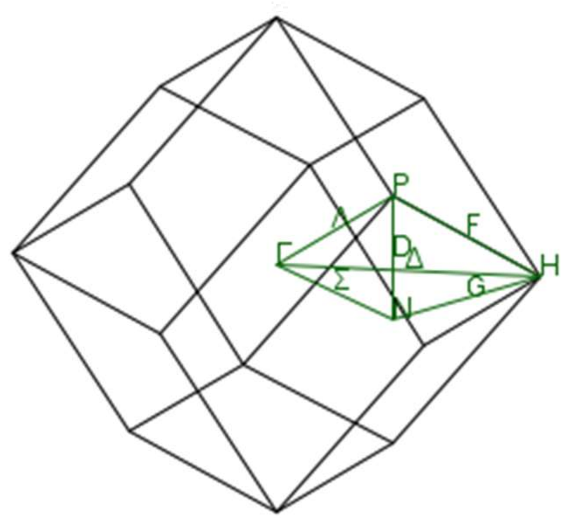


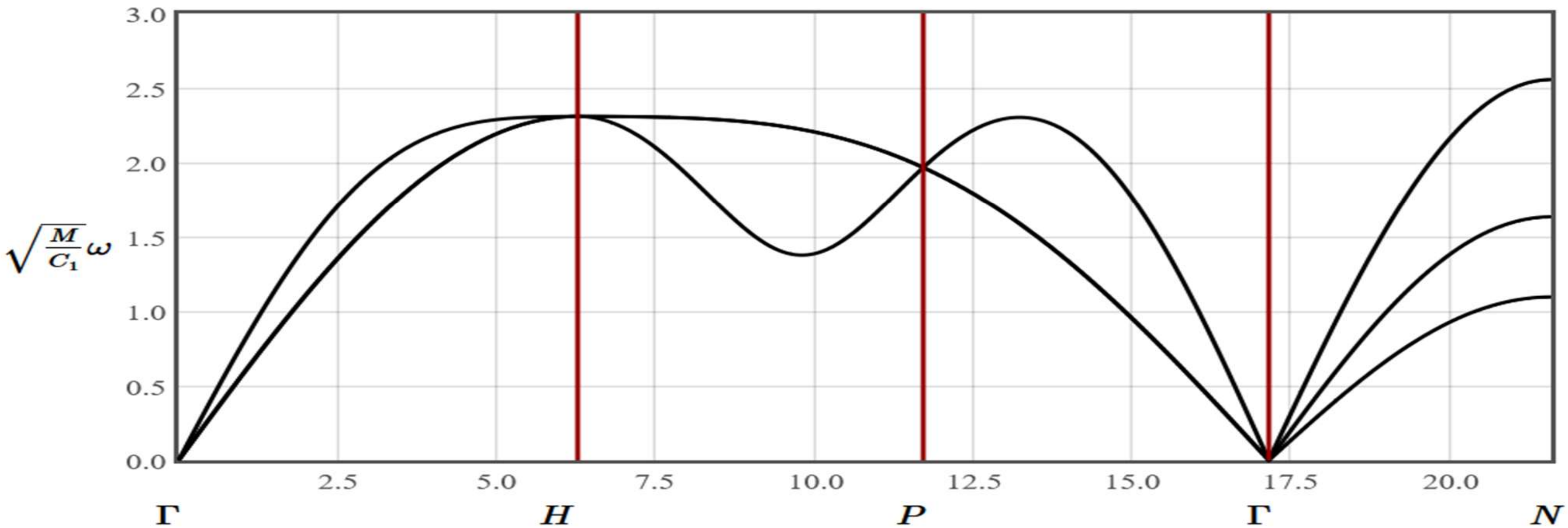


From Springer Materials: Landholt Boernstein Database

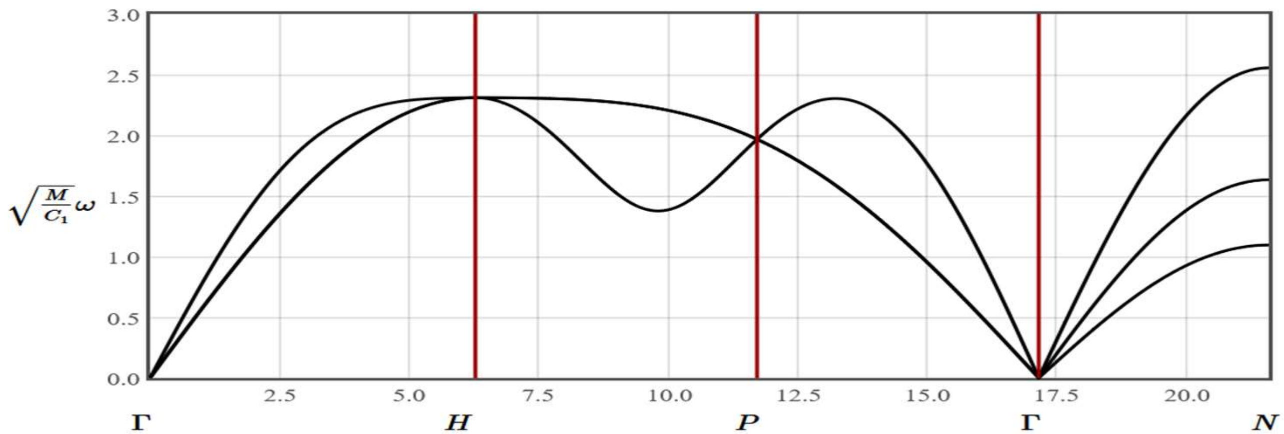
Phonon dispersion bcc

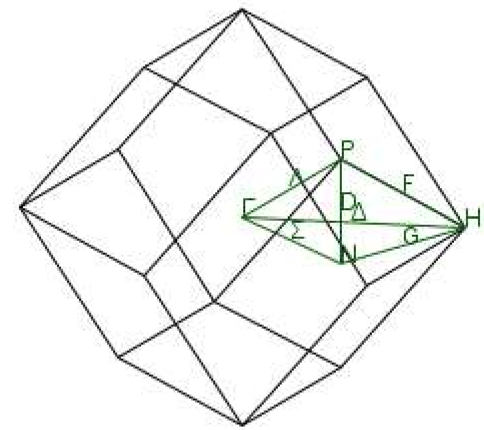






Phonon dispersion Fe





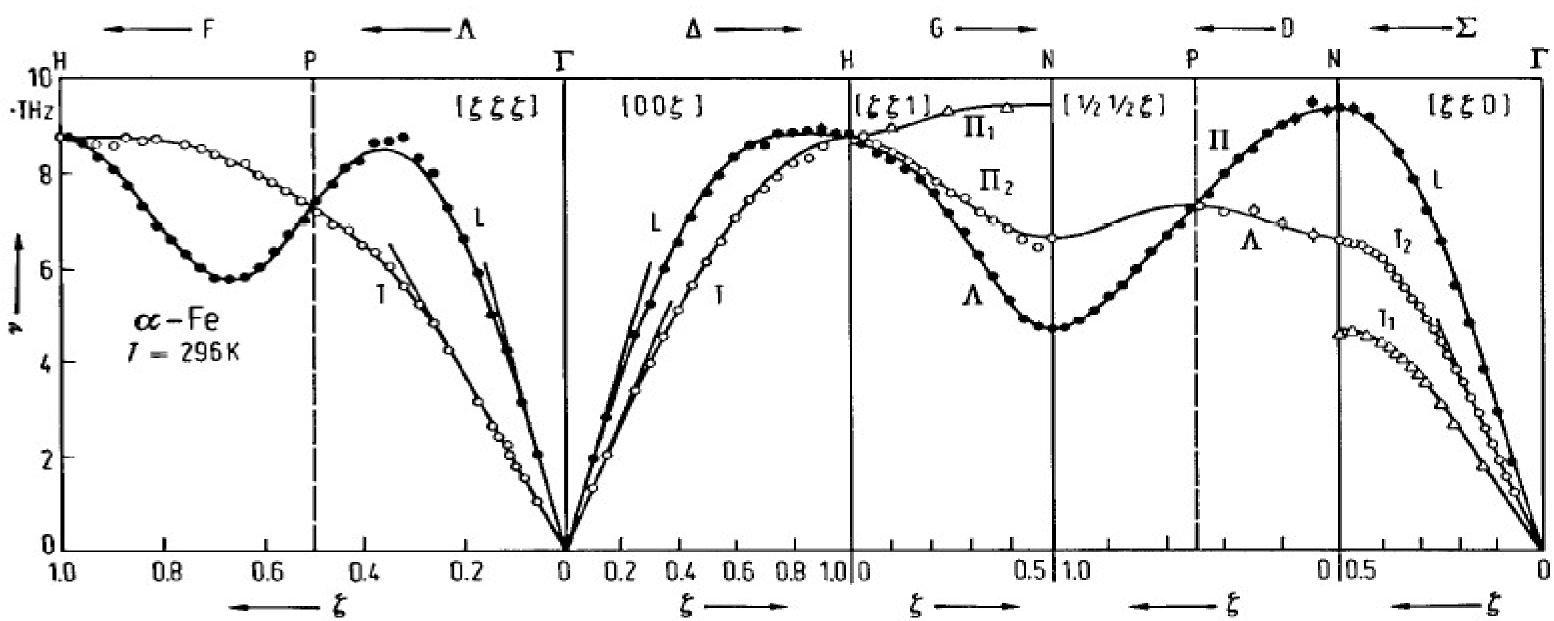
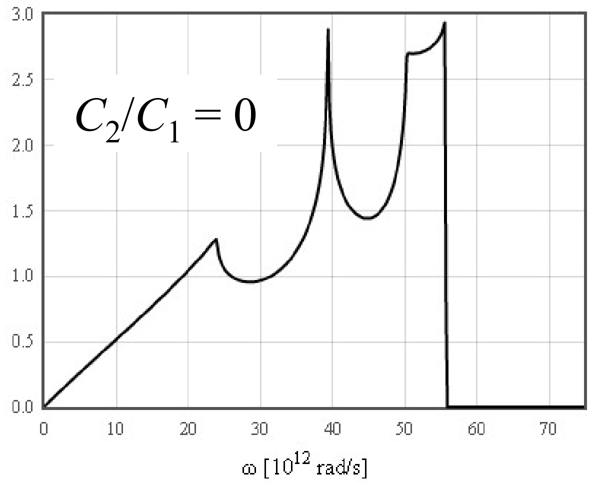


Fig. 2. Fe. Phonon dispersion curves in α-iron at 296 K. Experimental points: [68Va2]. Solid curve: fifth neighbour Born-von Karman model (Table 3 Fe [68Va2]).

From Springer Materials: Landholt Boernstein Database

Phonon DOS Fe

$D(\omega)$



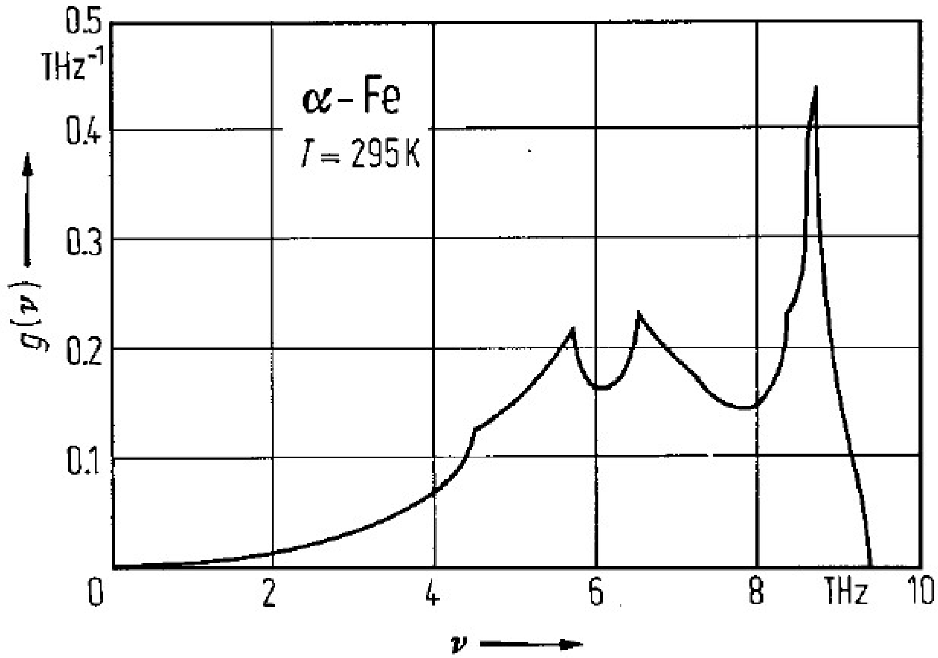
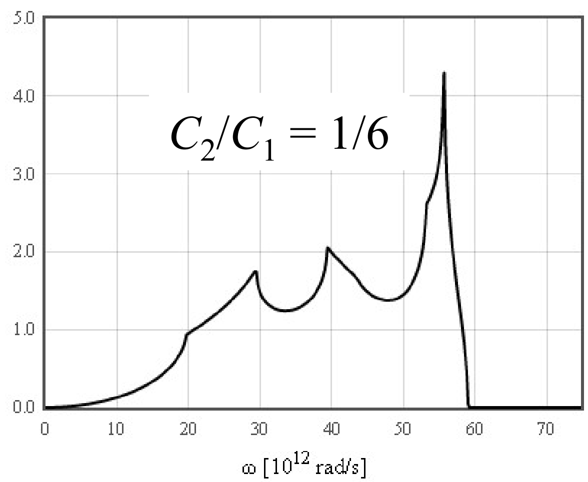


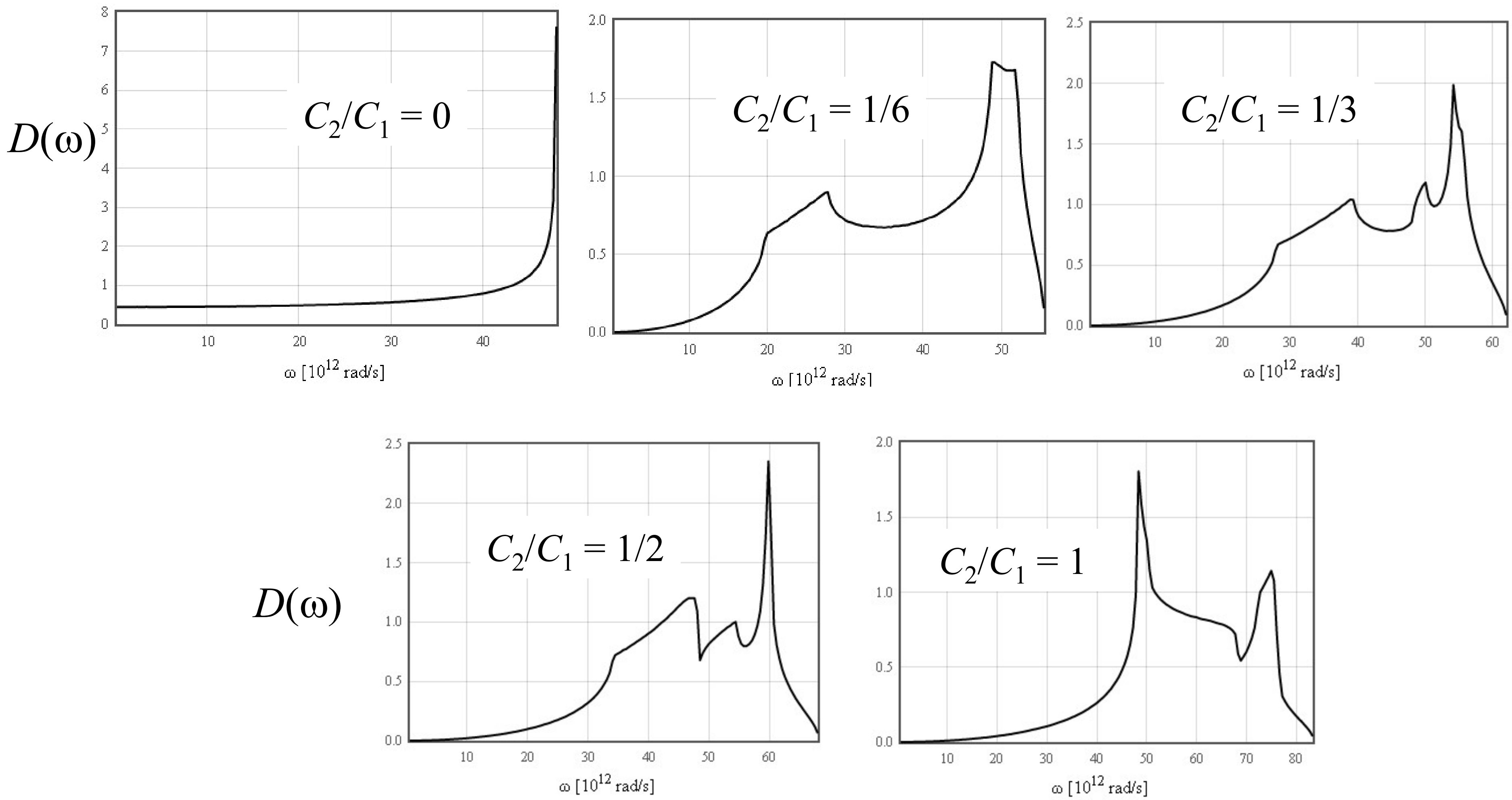
Fig. 3. Fe. Frequency spectrum of α-iron at 295 K calculated from the Born-von Karman force constants of Table 3 Fe [67Mi1].

$D(\omega)$



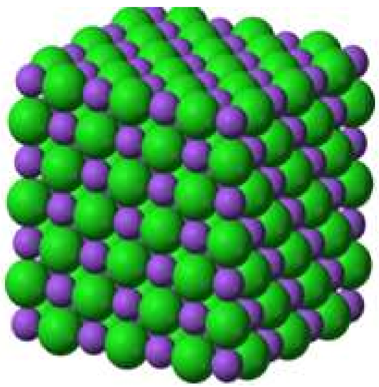
From Springer Materials: Landholt Boernstein Database

Next nearest neighbors (simple cubic)



Sometimes the 5th neighbors are included.

NaCl



2 atoms/unit cell

6 equations

3 acoustic and
3 optical branches

x - Richtung:

$$M_1 \frac{d^2 u^x_{nml}}{dt^2} = C\left(-2u^x_{nml} + v^x_{(n-1)m(l-1)} + v^x_{n(m-1)l}\right)$$

$$M_2 \frac{d^2 v^x_{nml}}{dt^2} = C\left(-2v^x_{nml} + u^x_{(n+1)m(l+1)} + u^x_{n(m+1)l}\right)$$

y - Richtung:

$$M_1 \frac{d^2 u^y_{nml}}{dt^2} = C\left(-2u^y_{nml} + v^y_{(n-1)(m-1)l} + v^y_{nm(l-1)}\right)$$

$$M_2 \frac{d^2 v^y_{nml}}{dt^2} = C\left(-2v^y_{nml} + u^y_{(n+1)(m+1)l} + u^y_{nm(l+1)}\right)$$

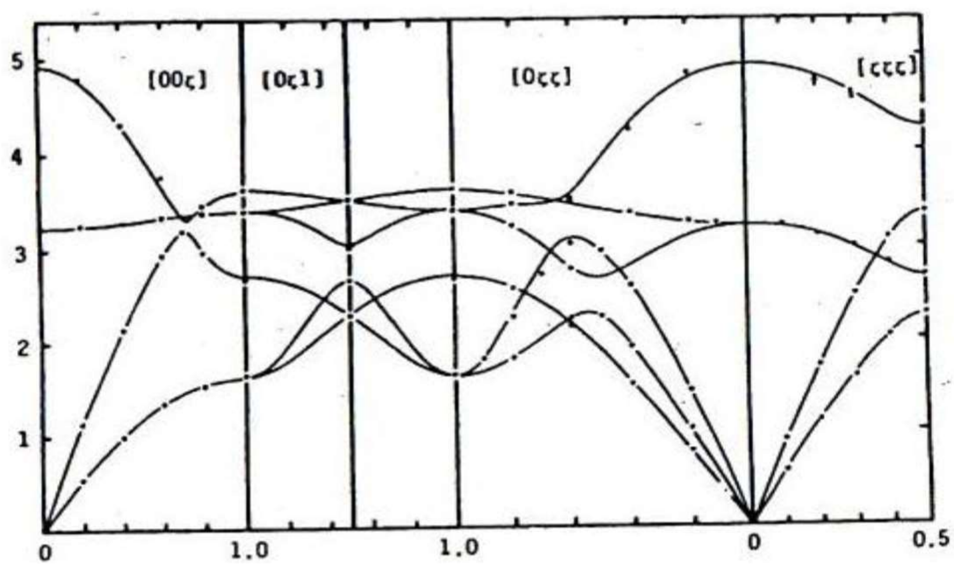
z - Richtung:

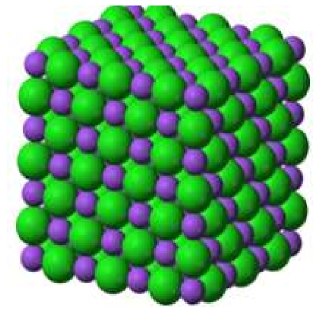
$$M_1 \frac{d^2 u^z_{nml}}{dt^2} = C\left(-2u^z_{nml} + v^z_{n(m-1)(l-1)} + v^z_{(n-1)ml}\right)$$

$$M_2 \frac{d^2 v^z_{nml}}{dt^2} = C\left(-2v^z_{nml} + u^z_{n(m+1)(l+1)} + u^z_{(n+1)ml}\right)$$

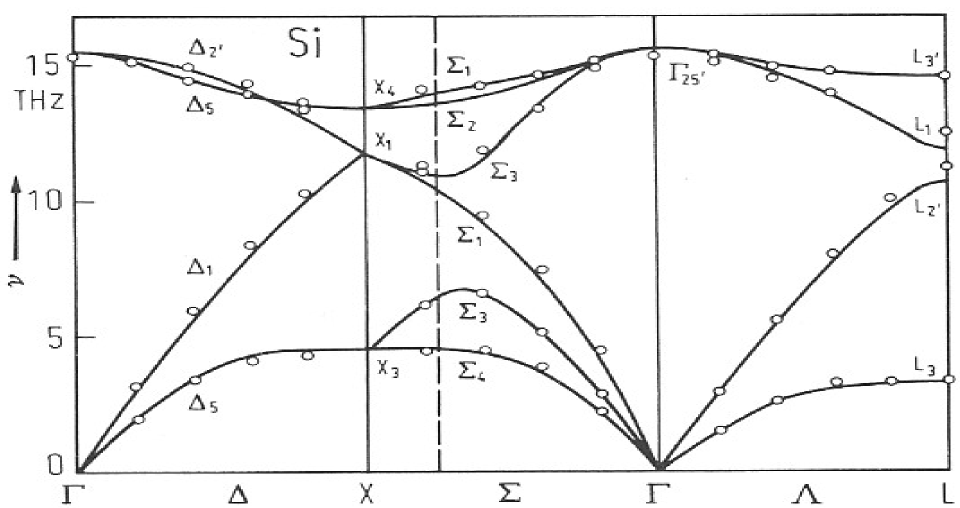
$$u^x_{nml} = u^x_{\vec{k}} \exp\left(i\left(\vec{k}\cdot\vec{a}_1 + \vec{k}\cdot\vec{a}_2 + \vec{k}\cdot\vec{a}_3 - \omega t\right)\right) \qquad v^x_{nml} = v^x_{\vec{k}} \exp\left(i\left(\vec{k}\cdot\vec{a}_1 + \vec{k}\cdot\vec{a}_2 + \vec{k}\cdot\vec{a}_3 - \omega t\right)\right)$$

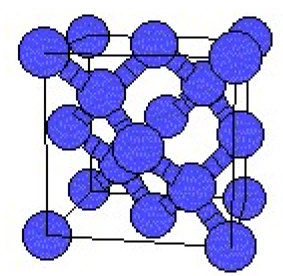
Two atoms per primitive unit cell





NaCl



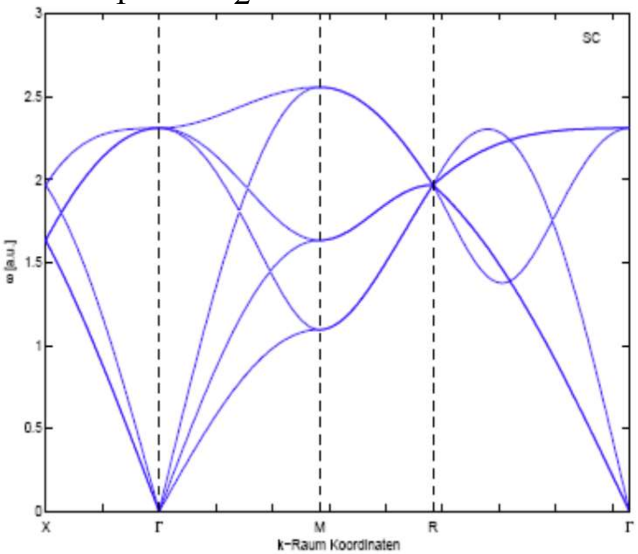


Si

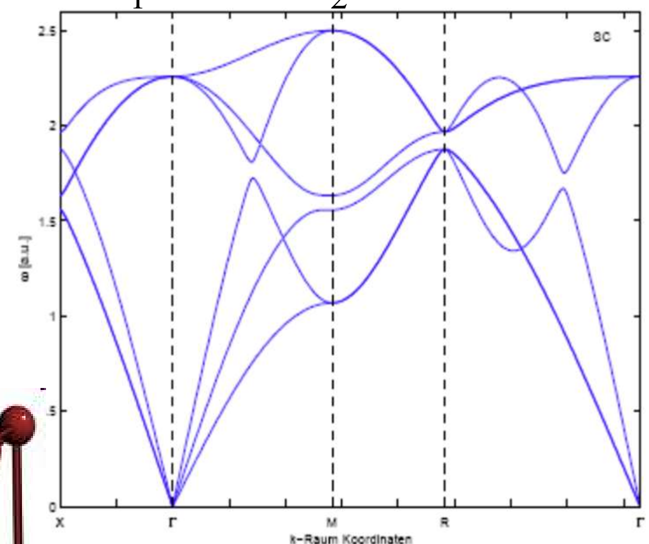
CsCl

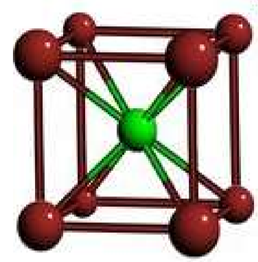
Hannes Brandner

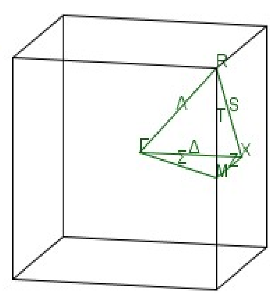
$M_1 = M_2$



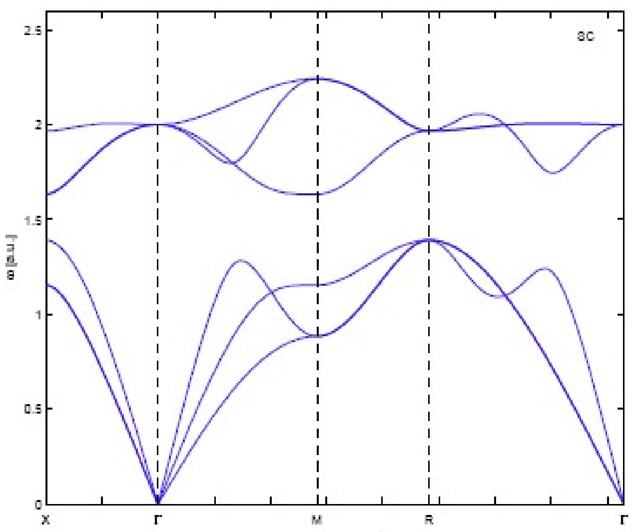
$M_1 = 1.1\ M_2$



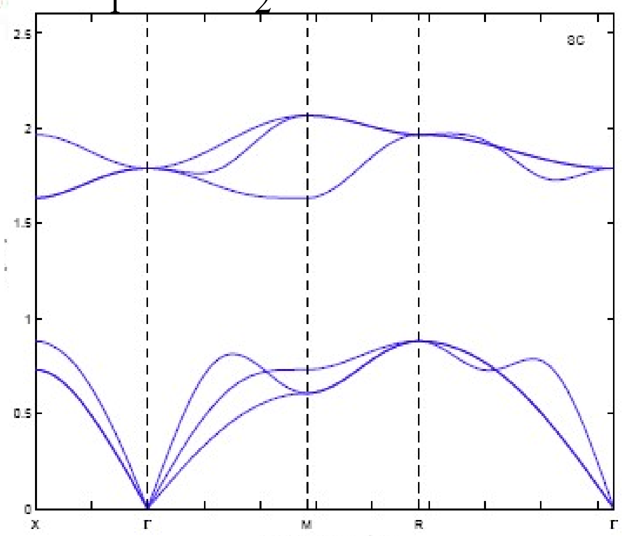




$M_1 = 2M_2$



$M_1 = 5M_2$



3 dimensions

N atoms

3*N* normal modes

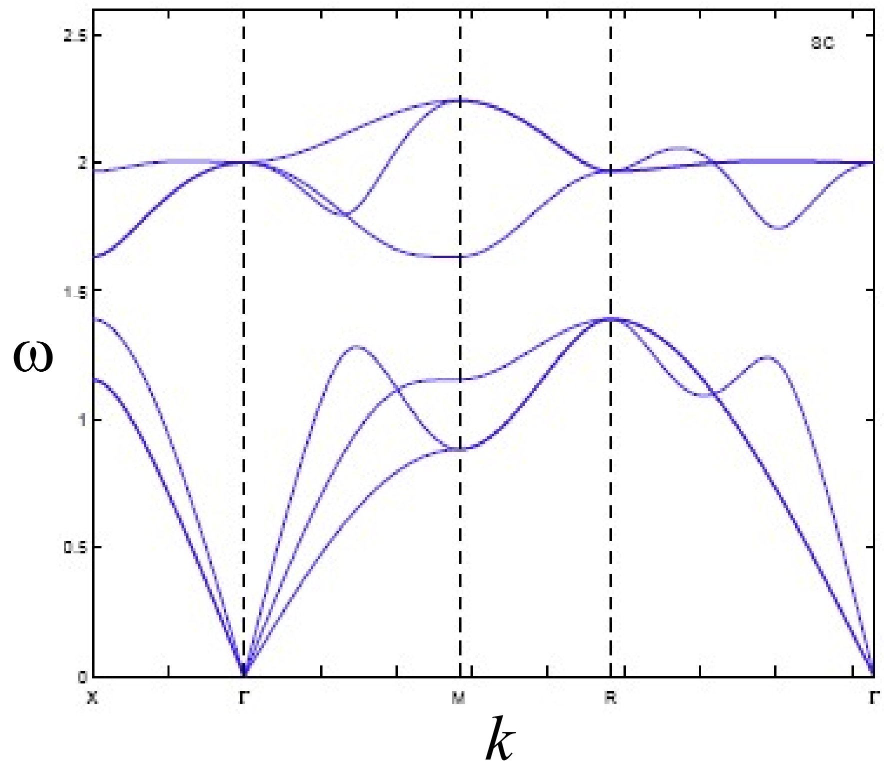
p atoms per unit cell

N/*p* unit cells = *k* vectors

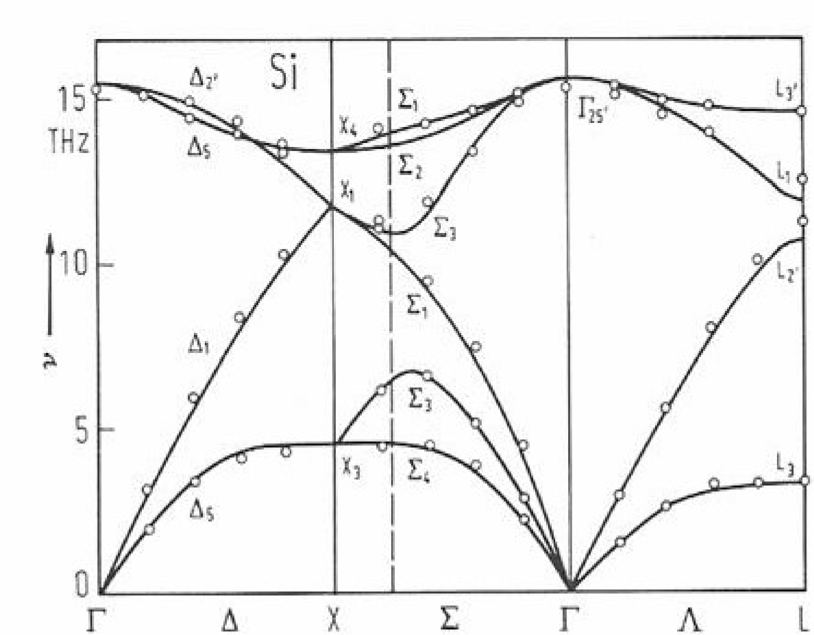
3*p* branches to the dispersion relation

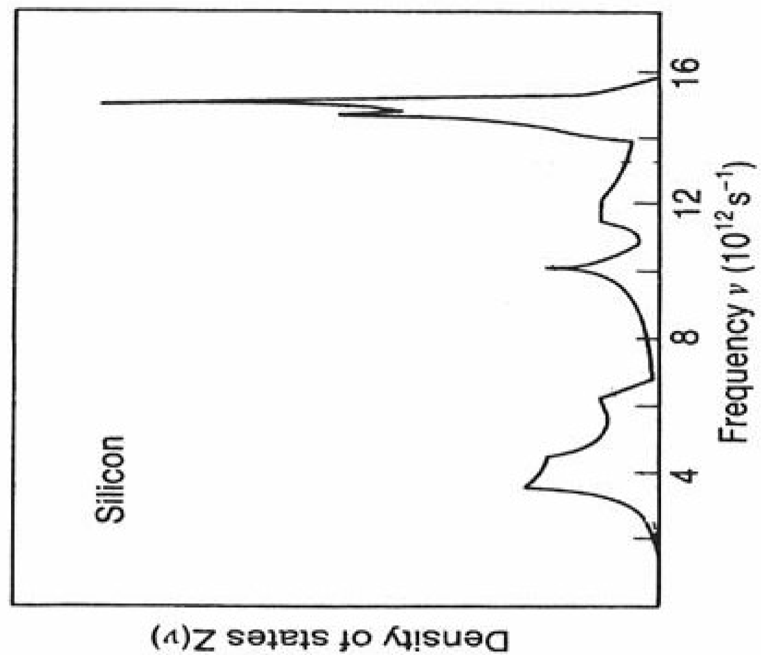
3 acoustic modes (1 longitudinal, 2 transverse)

3*p* - 3 optical modes

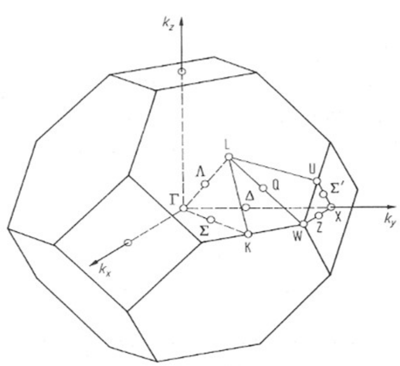


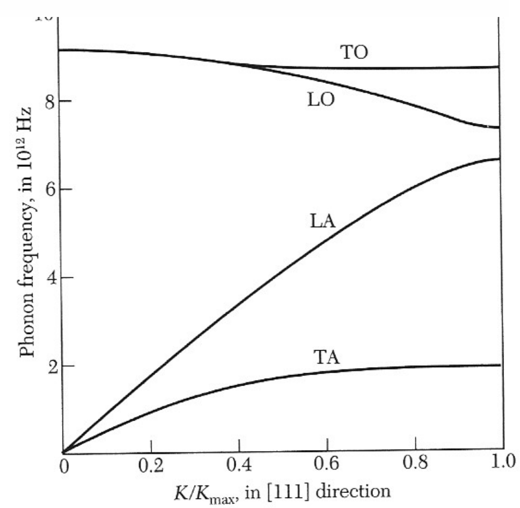
Silicon phonon dispersion, DOS



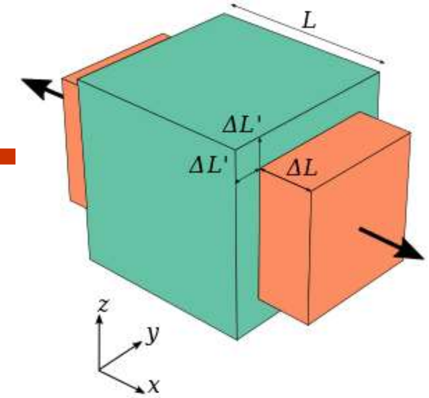


Different speeds of sound for different directions
and polarizations causes dispersion of pulses.





Poisson's ratio



Wikipedia

E - Elastic constant
ν - Poisson's ratio
ρ - density

$$c_T = \sqrt{\frac{E(1-\nu)}{\rho(1-\upsilon-2\upsilon^2)}}$$

$$c_L = \sqrt{\frac{E}{2\rho(1+\upsilon)}}$$

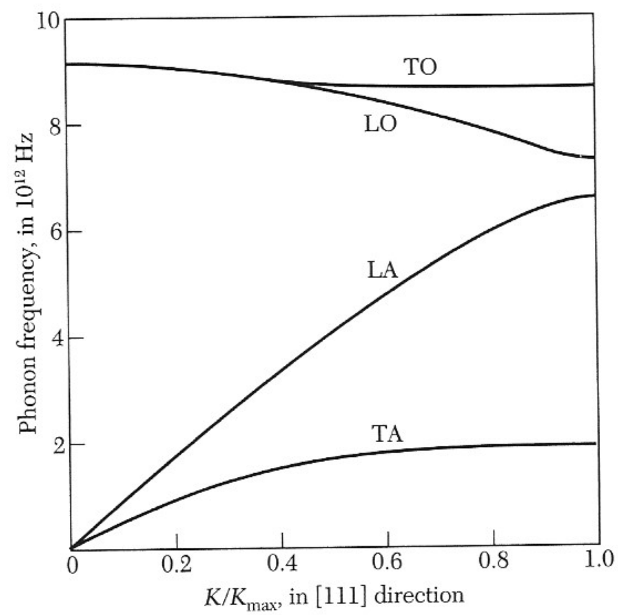
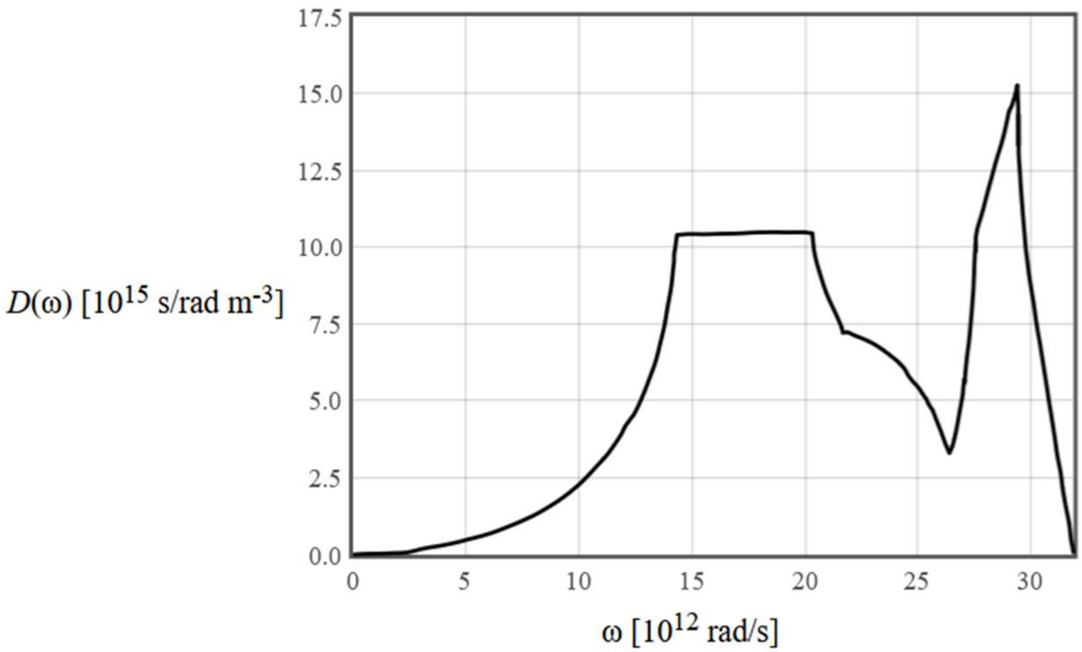


Figure 8a Phonon dispersion relations in the [111] direction in germanium at 80 K. The two TA phonon branches are horizontal at the zone boundary position, $K_{max} = (2\pi/a)(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The LO and TO branches coincide at $K = 0$; this also is a consequence of the crystal symmetry of Ge. The results were obtained with neutron inelastic scattering by G. Nilsson and G. Nelin.

Kittel

If the density is known, you can determine E and ν.

Phonon density of states for fcc silver



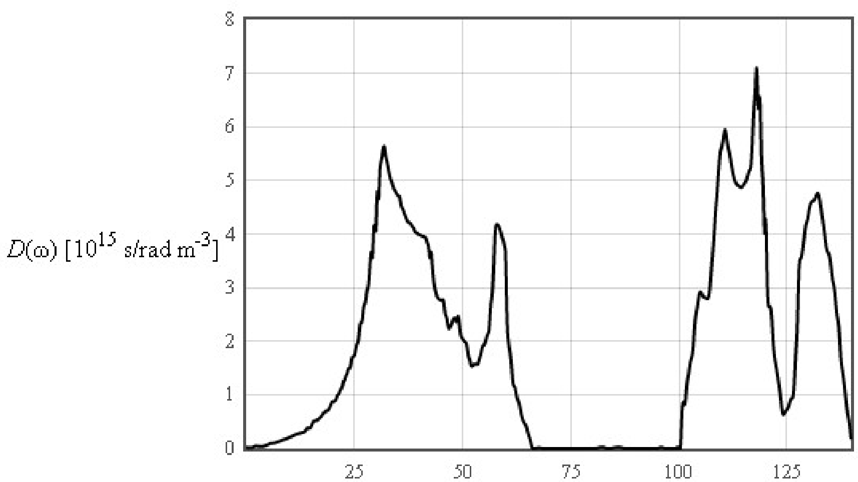
The atomic density is taken to be 5.86×10^{28} m^{-3}. Each atom has three degrees of freedom so the integral over all frequencies is $3\times5.86\times10^{28}$ m^{-3}. The data is from doi: 10.1007/b19988.

T = 296 K

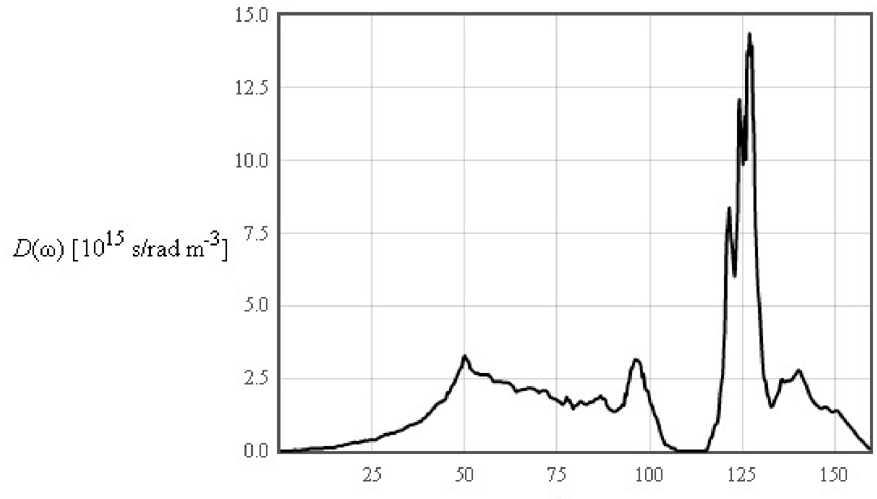
ω [rad/s]	$D(\omega)$ [s rad^{-1}m^{-3}]
0.0000	0.0000
5.7327e+10	6.8161e+12
4.0123e+11	2.3856e+13
7.4510e+11	3.0672e+13
1.0890e+12	3.4080e+13
1.4233e+12	4.0897e+13
1.7624e+12	5.1121e+13
2.0967e+12	5.7937e+13
2.4120e+12	7.4977e+13
2.7177e+12	1.2610e+14
3.0379e+12	1.8744e+14
3.3723e+12	2.3516e+14
3.7163e+12	2.7264e+14

Two atoms per primitive unit cell

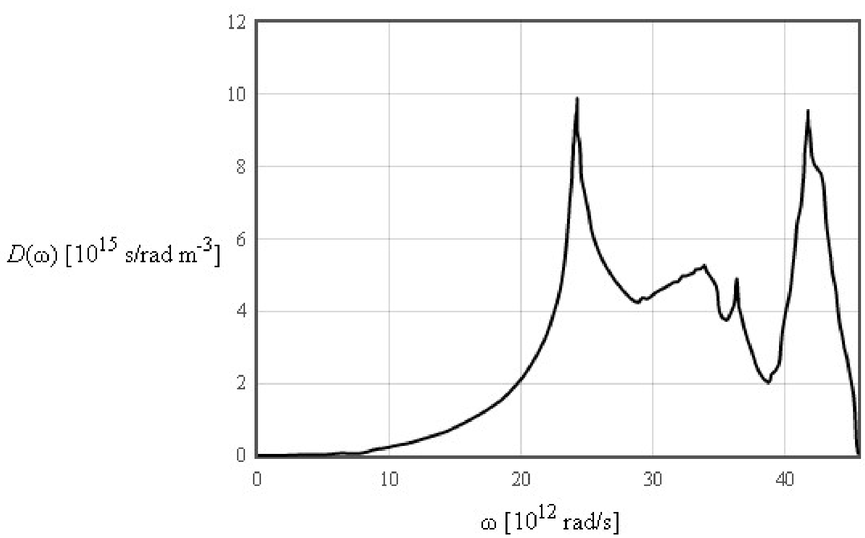
Phonon density of states for GaN



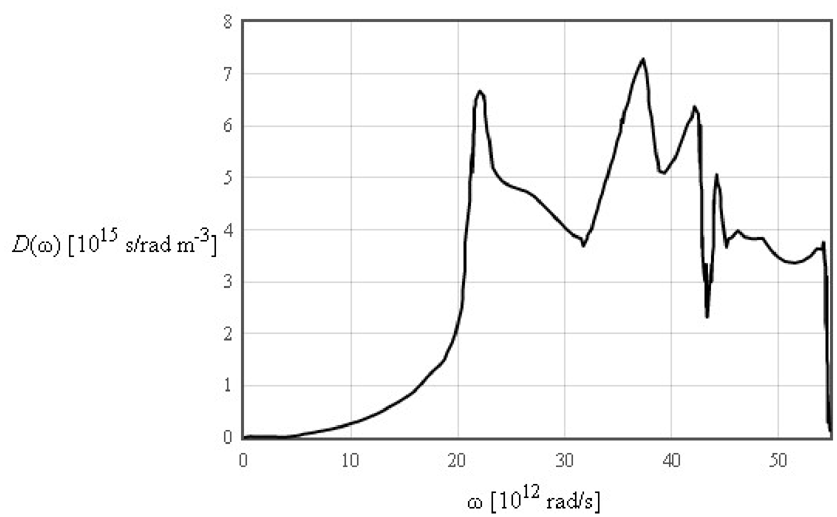
Phonon density of states for AlN

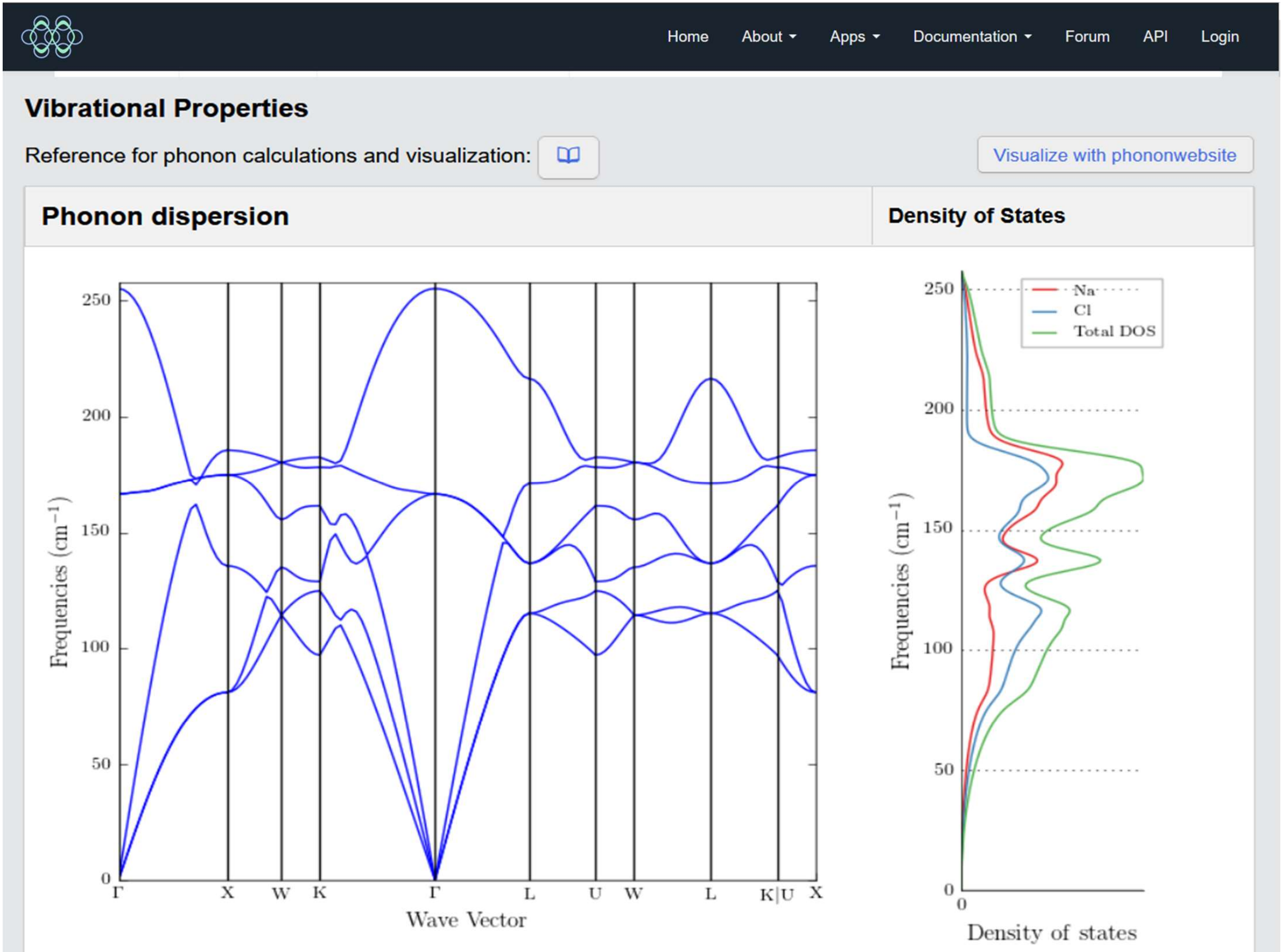


Phonon density of states for hcp magnesium



Phonon density of states for hcp titanium

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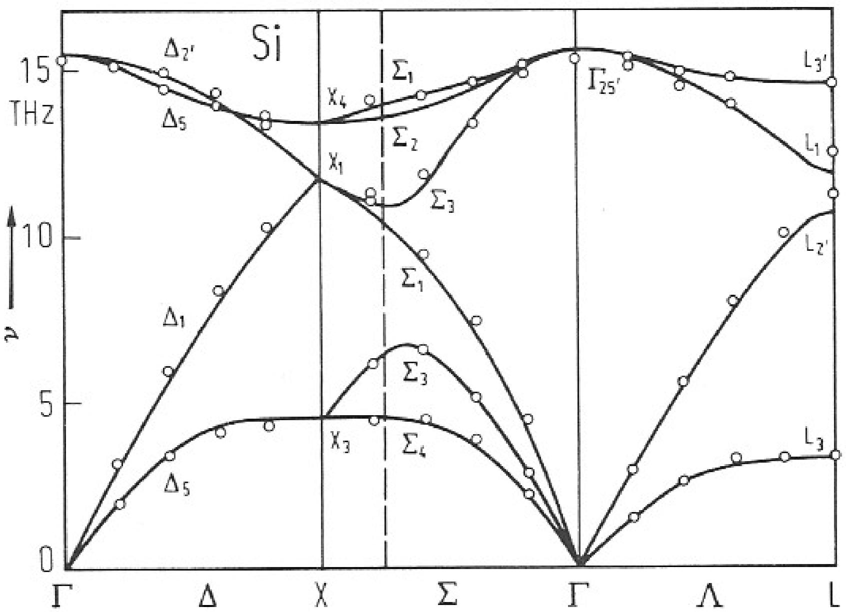
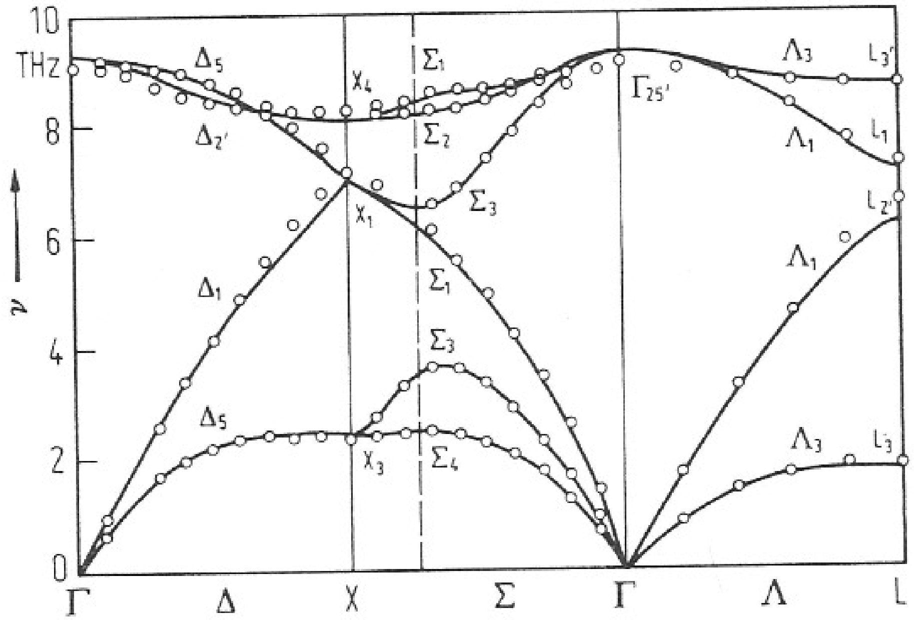
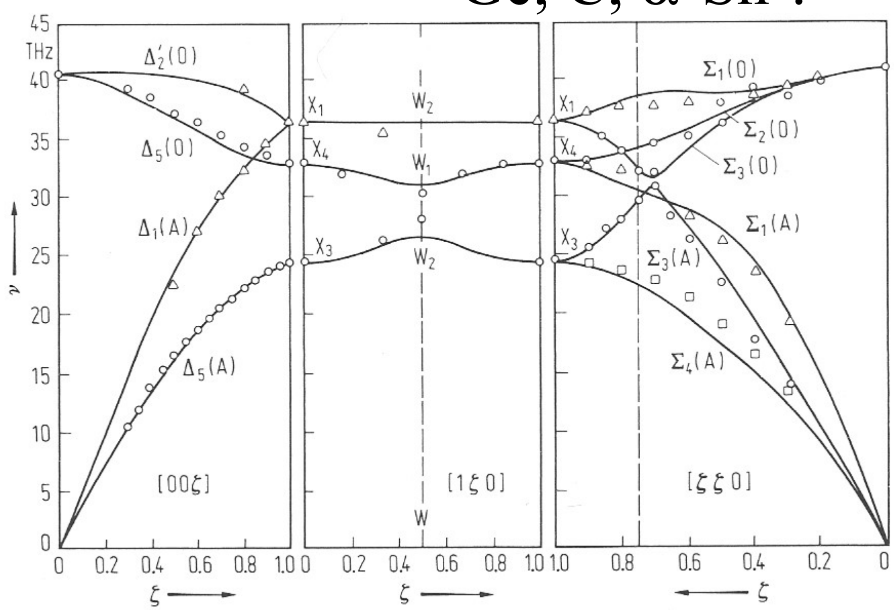
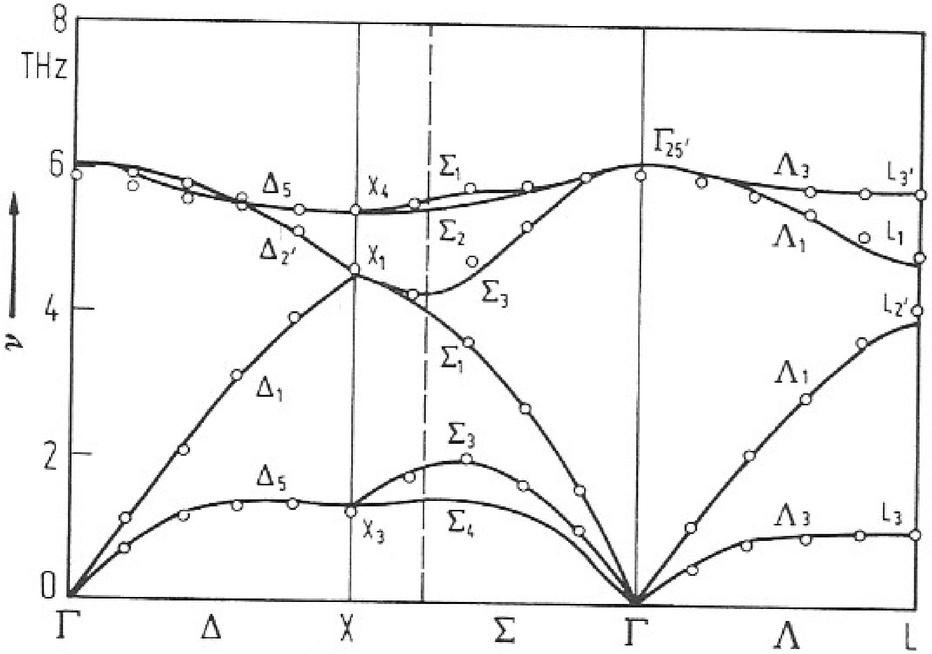
Reference for phonon calculations and visualization:
Visualize with phononwebsite
Phonon dispersion
Density of States
Frequencies (cm⁻¹)
250
200
150
100
50
0
Γ X W K Γ L U W L K|U X
Wave Vector
Na
Cl
Total DOS
Density of states


Si
15
THz
10
5
0
ν
Γ
Δ
X
Σ
Γ
Λ
L
Δ2'
Δ5
Δ1
Δ5
X4
X1
X3
Σ1
Σ2
Σ3
Σ1
Σ3
Σ4
Γ25'
L3'
L1
L2'
L3


10
THz
8
6
4
2
0
ν
Γ
Δ
X
Σ
Γ
Λ
L
Δ5
Δ2'
Δ1
Δ5
X4
X1
X3
Σ1
Σ2
Σ3
Σ1
Σ3
Σ4
Γ25'
Λ3
Λ1
Λ1
Λ3
L3'
L1
L2'
L3

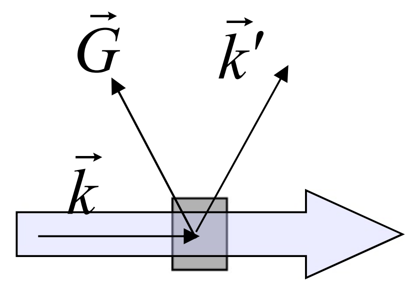
Ge, C, α-Sn ?


45
THz
40
35
30
25
20
15
10
5
0
ν
Δ'2(O)
Δ5(O)
Δ1(A)
Δ5(A)
X1
X4
X3
W2
W1
W2
W
Σ1(O)
Σ2(O)
Σ3(O)
Σ1(A)
Σ3(A)
Σ4(A)
[00ζ]
[1ζ0]
[ζζ0]
0 0.2 0.4 0.6 0.8 1.0
0 0.2 0.4 0.6 0.8 1.0
1.0 0.8 0.6 0.4 0.2 0
ζ
ζ
ζ


8
THz
6
4
2
0
ν
Γ
Δ
X
Σ
Γ
Λ
L
Δ5
Δ2'
Δ1
Δ5
X4
X1
X3
Σ1
Σ2
Σ3
Σ1
Σ3
Σ4
Γ25'
Λ3
Λ1
Λ1
Λ3
L3'
L1
L2'
L3

Inelastic neutron scattering

Diffraction condition for elastic scattering



$$\vec{k}' = \vec{k} + \vec{G}$$

The whole crystal recoils with momentum $\hbar\vec{G}$

Diffraction condition for inelastic scattering

$$\vec{k}' \pm \vec{K}_{ph} = \vec{k} + \vec{G} \qquad \frac{\hbar^2 k'^2}{2m_n} \pm \hbar\omega_{ph} = \frac{\hbar^2 k^2}{2m_n} + \cancelto{0}{\frac{\hbar^2 G^2}{2m_{crystal}}}$$

$\vec{K}_{ph}$ is the phonon momentum

Phonon dispersion relations are determined experimentally by inelastic neutron diffraction

long wavelength limit

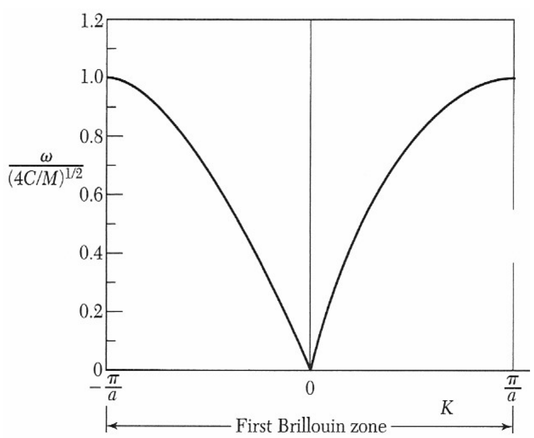
discrete version of wave equation

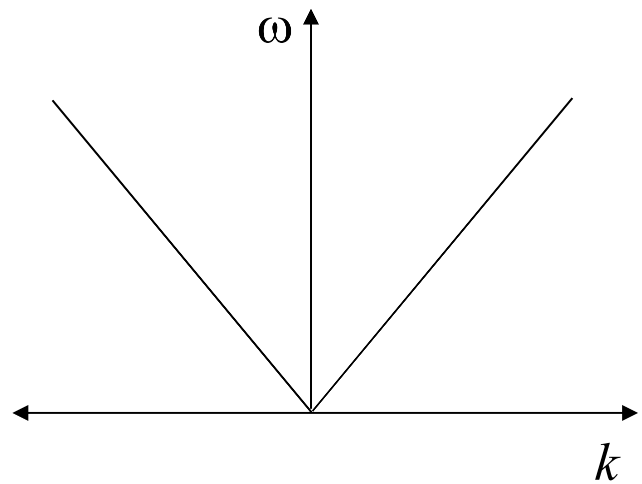
$$m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$

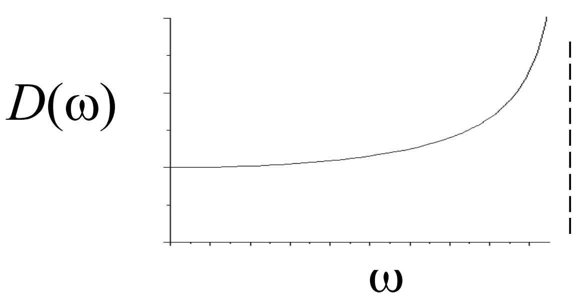
1-d wave equation

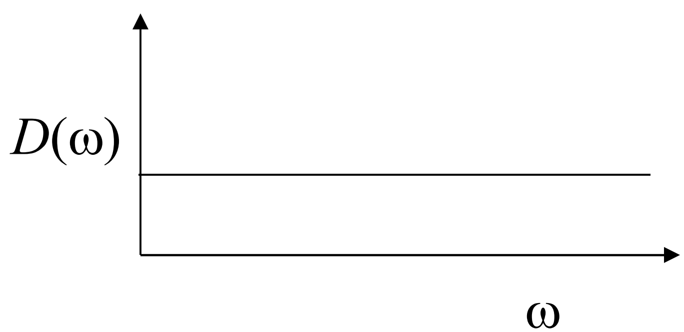
$$\frac{d^2u}{dt^2} = c^2\frac{d^2u}{dx^2}$$

The solutions to the linear chain are the same as the solutions to the wave equation for $|k| << \pi/a$.

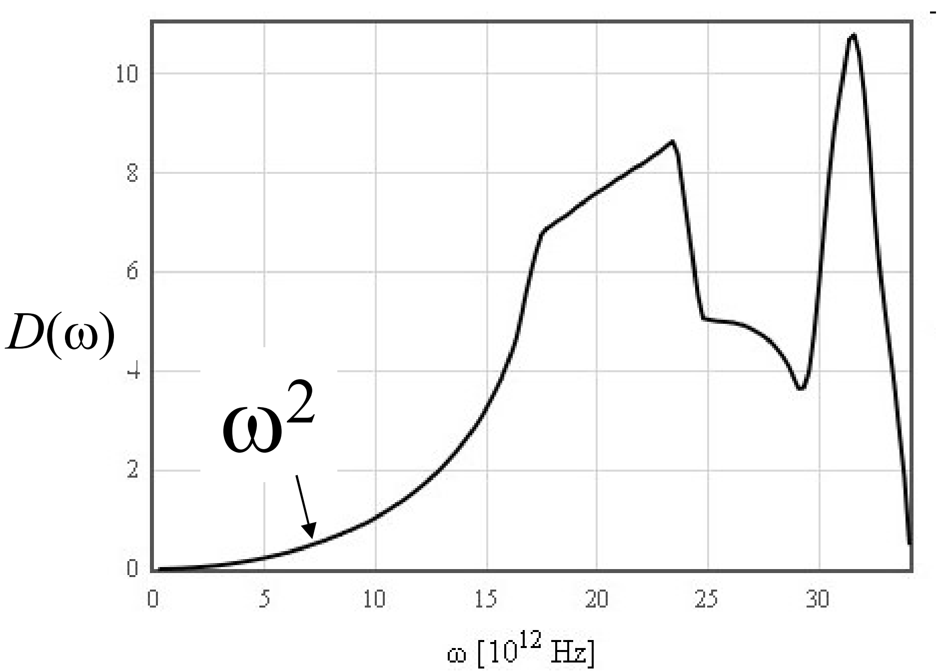


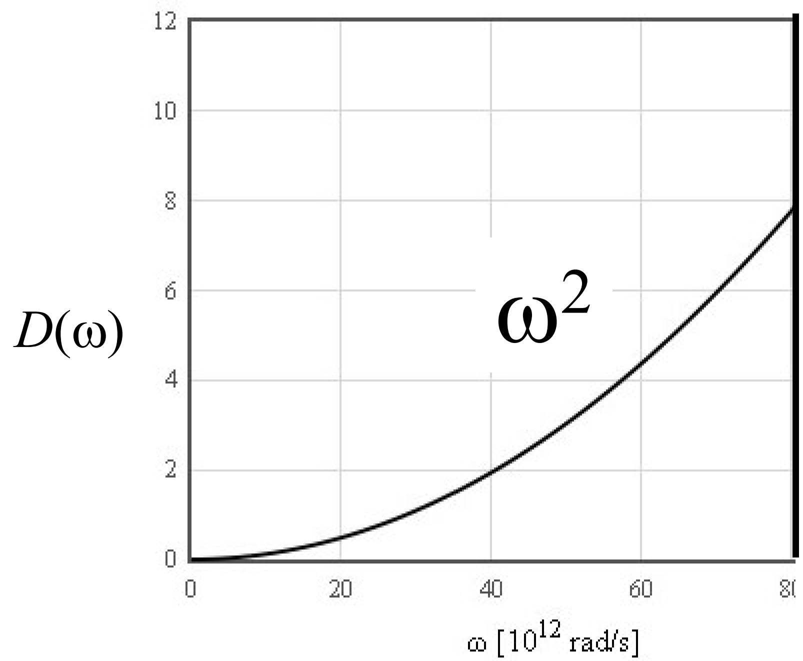






long wavelength limit





Phonons - long wavelength, low temperature limit

At low T, there are only long wavelength states occupied.

3 polarizations

Density of states: $$D(\omega)d\omega = \frac{3\omega^2}{2c^3\pi^2}d\omega.$$

Specific heat of insulators at low temperatures

$$C_v = \frac{24\sigma V T^3}{c}$$

Speed of sound

$$I = \frac{2\pi^5 k_B^4 T^4}{15 c^2 h^3} = \sigma T^4 \quad [\mathrm{J\ m^{-2}\ s^{-2}}]$$

$$u(\lambda) = \frac{8\pi hc}{\lambda^5\left(\exp\left(\frac{hc}{\lambda k_B T}\right)-1\right)} \quad [\mathrm{J/m^4}]$$

$$u = \frac{4\sigma T^4}{c} \quad [\mathrm{J/m^3}]$$

$$c_v = \frac{16\sigma T^3}{c} \quad [\mathrm{J\ K^{-1}\ m^{-3}}]$$

$$f = \frac{-4\sigma T^4}{3c} \quad [\mathrm{J/m^3}]$$

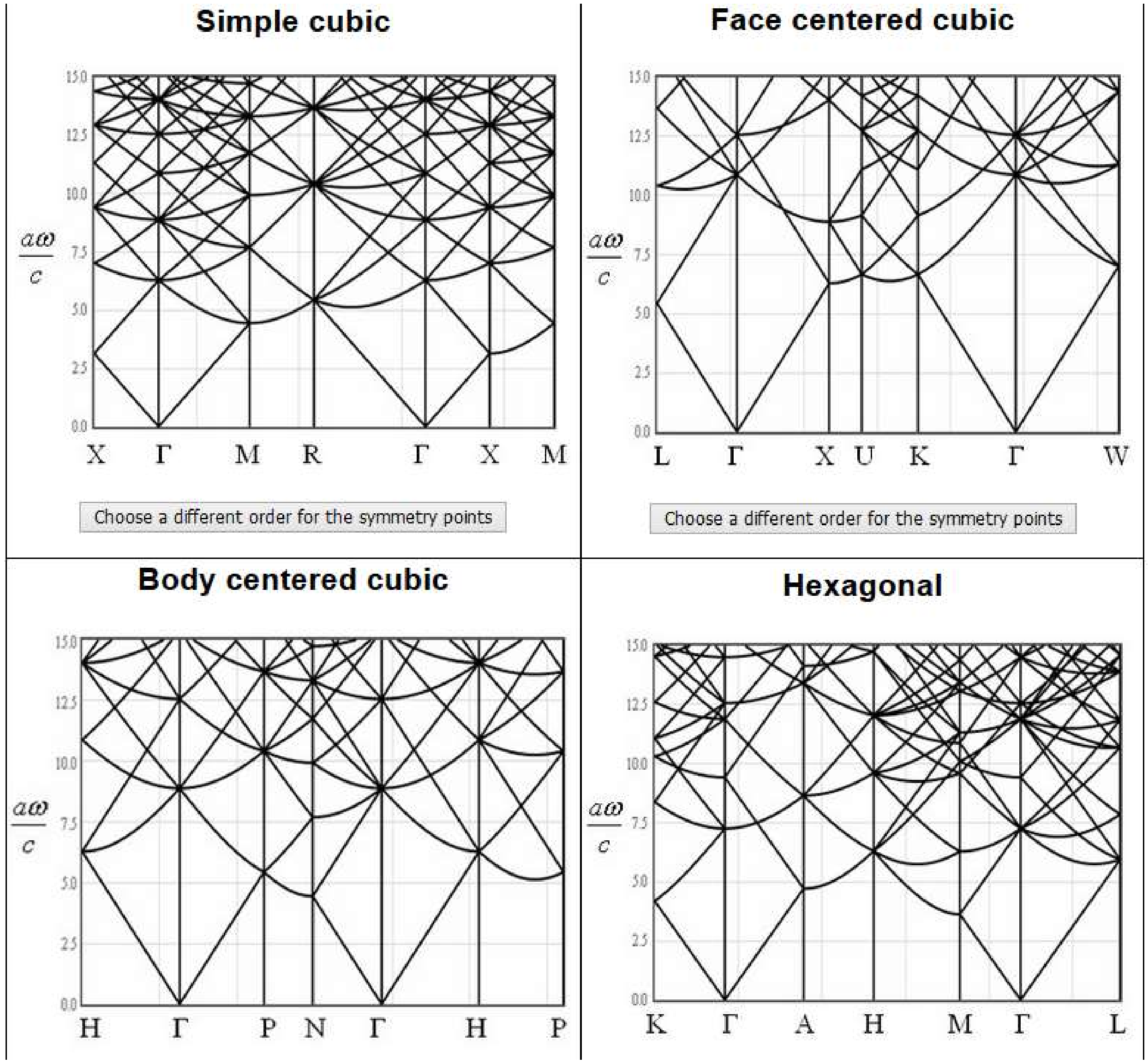
$$s = \frac{16\sigma T^3}{3c} \quad [\mathrm{J\ K^{-1}\ m^{-3}}]$$

$$P = \frac{4\sigma T^4}{3c} \quad [\mathrm{N/m^2}]$$

Empty lattice approximation

Use the speed of sound instead of the speed of light.

3 acoustic branches
3p - 3 optical branches



Thermal properties

1. **Determine the dispersion relation:**

   Write down the equations of motion (masses and springs).

   The solutions to these equations will be eigen functions of **T**

$$\exp\left(i\left(\vec{k}\cdot\vec{a}_1+\vec{k}\cdot\vec{a}_2+\vec{k}\cdot\vec{a}_3-\omega t\right)\right)$$

   Substitute the eigen functions of **T** into the equations of motion to determine the dispersion relation.

2. **Determine the density of states numerically from the dispersion relation** $D(\omega)$

   For every allowed *k*, find all corresponding values of ω.

Specific Heat

$$u(T) = \int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$

$$c_v = \left(\frac{\partial u}{\partial T}\right)_{N,V}$$

$$c_v = \int \hbar\omega D(\omega) \frac{\partial}{\partial T} \left(\frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}\right) d\omega$$

$$c_v = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega) e^{\frac{\hbar\omega}{k_B T}}}{k_B \left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^2} d\omega$$

http://lampx.tugraz.at/~hadley/ss1/phonons/table/dos2cv.html

Heat capacity / specific heat

Heat capacity is the measure of the heat energy required to increase the temperature of an object by a certain temperature interval.

Specific heat is the measure of the heat energy required to increase the temperature of a unit quantity of a substance by a certain temperature interval.

For solids, the heat capacity at constant volume and heat capacity at constant pressure are almost the same.

The heat capacity was historically important for understanding solids.

Dulong and Petit (Classical result)

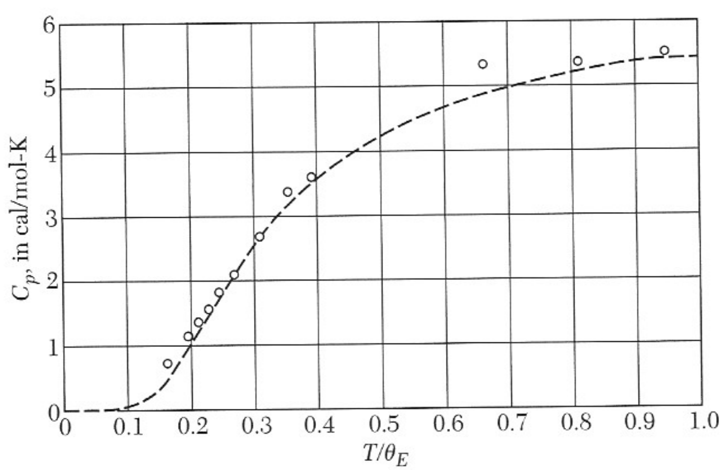
Equipartition: $\frac{1}{2}k_B T$ per quadratic term in energy

internal energy: $u = 3nk_B T$ n = atomic density

specific heat: $c_v = \frac{du}{dT} = 3nk_B$

experiments: heat capacity goes to zero at zero temperature


Pierre Louis Dulong




Alexis Therese Petit