Solid State Theory: Band Structure Methods

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Computer room

http://itp.tugraz.at/LV/boeri/ELE/

Outline:

- Computing the phonon frequencies of silicon at the Gamma point.
- Generating a grid in q space.
- Computing the frequencies of silicon on a regular grid.
- Obtaining dispersions through Fourier transform of the force constants.

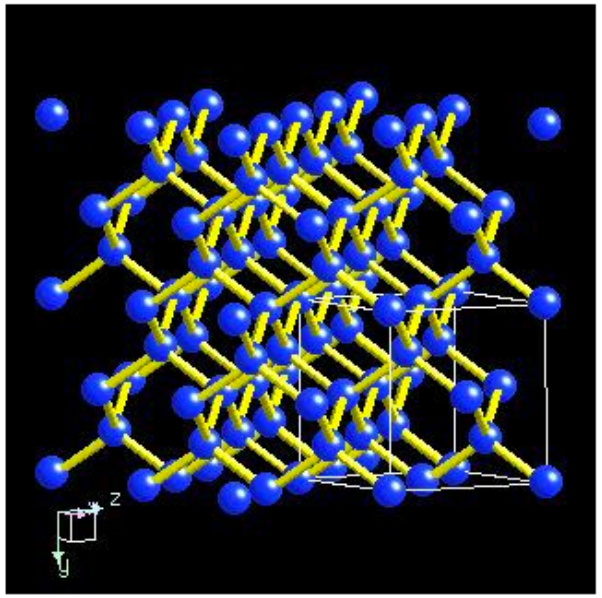
http://www.quantum-espresso.org/

Silicon:

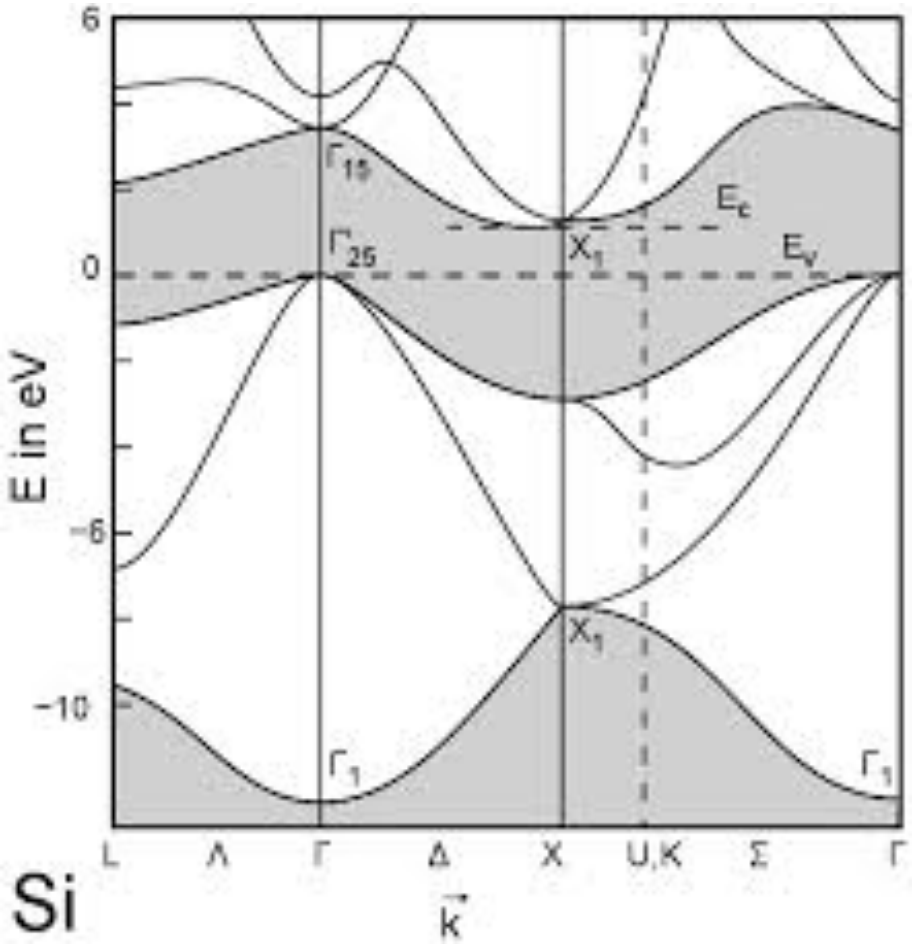
Table: basic information about and classifications of silicon.

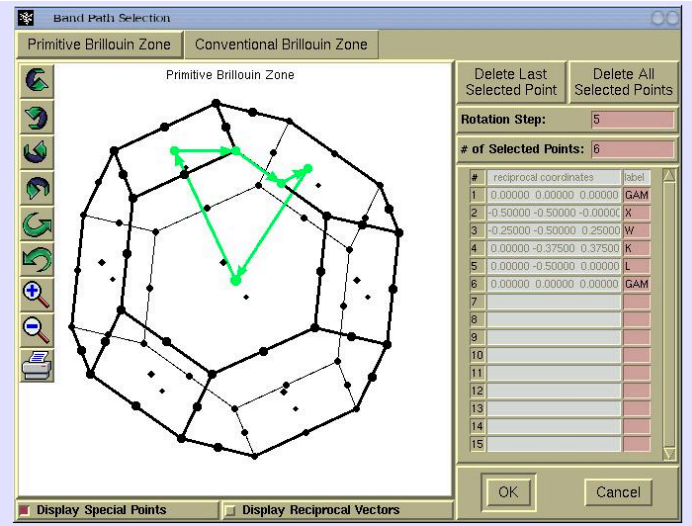
- Name: Silicon
- Symbol: Si
- Atomic number: 14
- Atomic weight: 28.0855 (3) [see note r]
- Standard state: solid at 298 K
- CAS Registry ID: 7440-21-3
- Group in periodic table: 14
- Group name: (none)
- Period in periodic table: 3
- Block in periodic table: p-block
- Colour: dark grey with a bluish tinge
- Classification: Semi-metallic

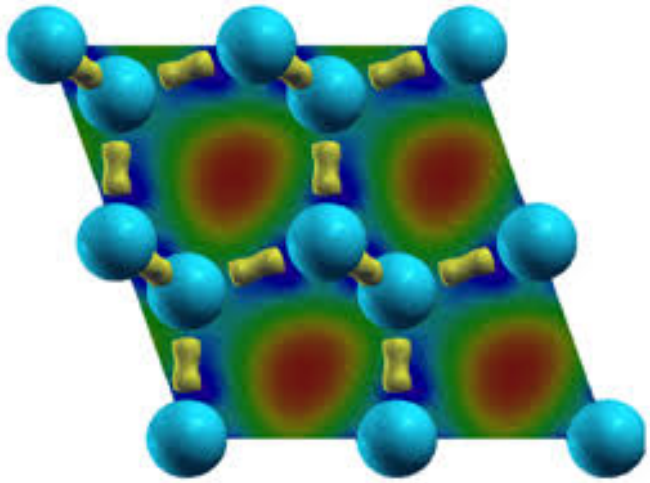
Space group: Fd-3m (Space group number: 227)
Structure: diamond
Cell parameters:
a: 543.09 pm
b: 543.09 pm
c: 543.09 pm
α: 90.000°
β: 90.000°
γ: 90.000°



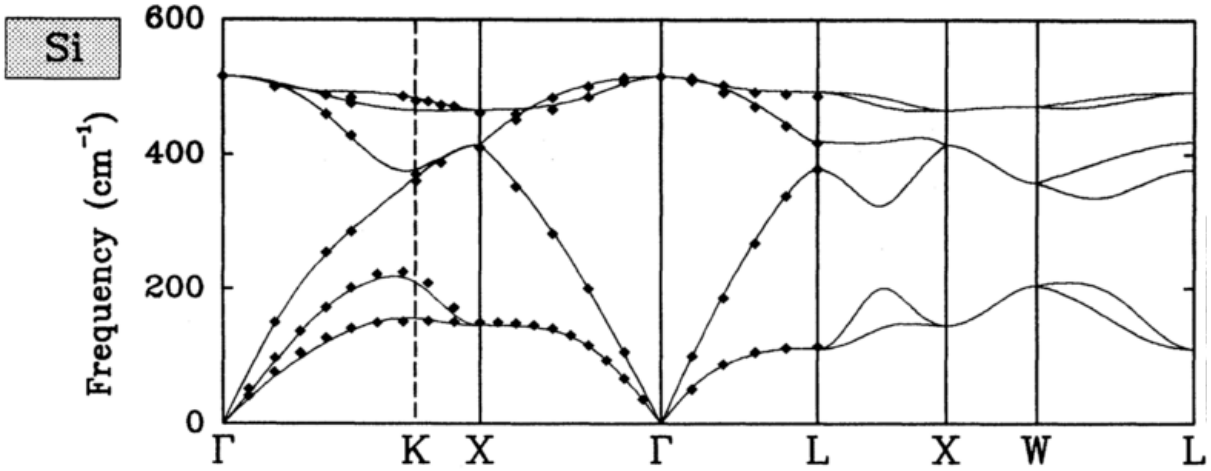
Electronic Structure:







Silicon Phonon Dispersions

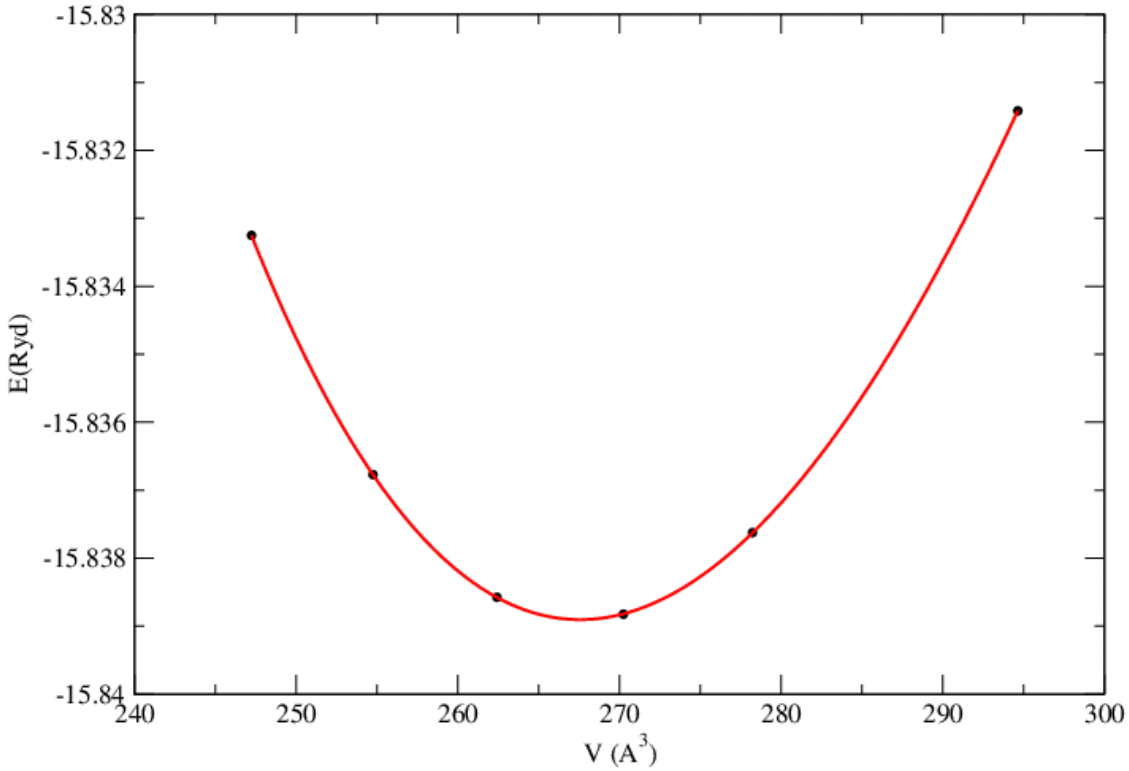


Q point	Ω (THz)
$\Gamma_{LO/TO}$	15.5
X_{TO}	13.9
$X_{LA/TO}$	12.3
X_{TA}	4.5
L_{TO}	14.7
L_{LO}	12.6
L_{LA}	11.4
L_{TA}	3.4

Units:

1THz=33.357 cm^{-1}=122.65 meV

Equation of state:



Equation of state: EOS2 (PRB52,8064)

a,b,c,d -15.977229 52.489842 -659.228070 2105.431619

V0,B(GPa),BP,E0 267.5514 94.4139 4.0179

Equation of state: Murnaghan

V0,B(GPa),BP,E0 267.5519 94.1350 4.0339 -15.838904

Experiment:

V0,B(GPa): 270.24 97.6

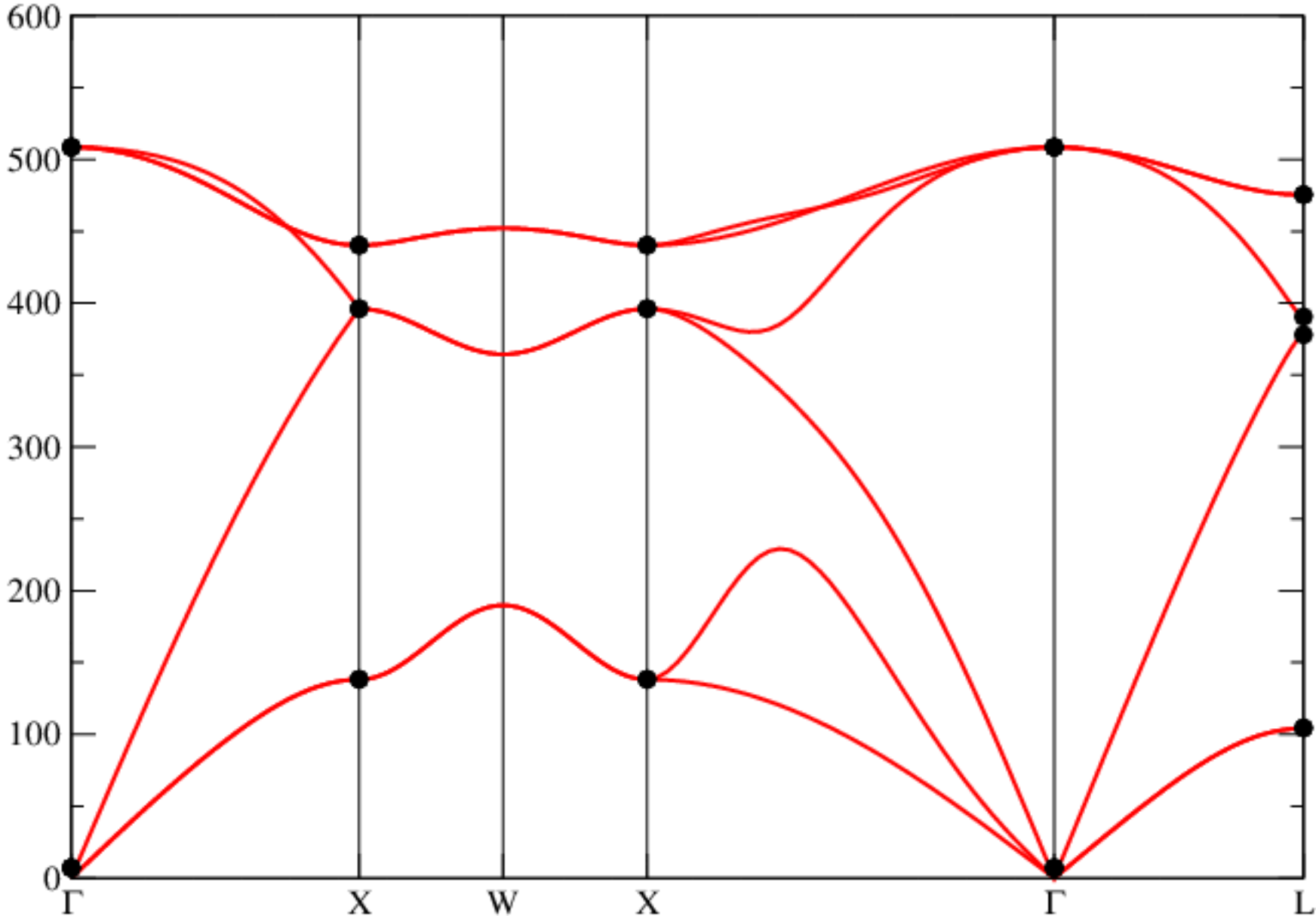
Pressure Behaviour (Gruneisen Parameters):

$$\gamma_i = \frac{B_T}{\omega_i}\frac{\partial \omega_i}{\partial P}$$

Table I. Mode Grüneisen parameter γ_i for Si and Ge.

Γ	Si	Ge	L	Si	Ge
$\gamma_{TO}(=\gamma_{LO})$	1.00 ± 0.06	1.12 ± 0.02	γ_{TO}	1.3 ± 0.2	0.9 ± 0.1
$\gamma_{LA}[1,0,0]$	1.110	1.301	γ_{LO}	1.2*	1.2 ± 0.2
$\gamma_{TA}[1,0,0]$	0.325	0.612	γ_{LA}	1.0*	0.5 ± 0.1
$\gamma_{LA}[1,1,0]$	1.106	1.294	γ_{TA}	-1.3 ± 0.3	-0.4 ± 0.3
$\gamma_{TA_1}[1,1,0]$	0.325	0.612	X		
$\gamma_{TA_2}[1,1,0]$	-0.099	0.161	γ_{TO}	1.5 ± 0.1	——
$\gamma_{LA}[1,1,1]$	1.105	1.292	$\gamma_{LO}(\simeq\gamma_{LA})$	0.9*	——
$\gamma_{TA}[1,1,1]$	0.086	0.367	γ_{TA}	-1.4 ± 0.3	——

* These data are adopted as the average value in many theories[6–11] and bring only a little influence on the total Grüneisen constant.


600
500
400
300
200
100
0
Γ
X
W
X
Γ
L