Second Lecture

Separate atoms Bands

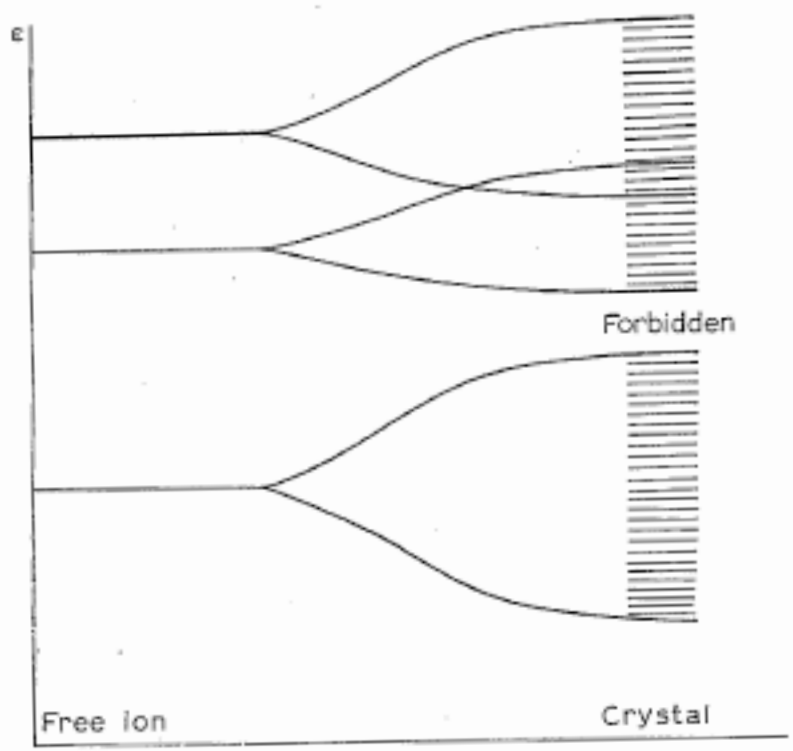


Fig. 4.1. Schematic broadening of one-electron energy levels for a free ion into bands when the ion is incorporated in a crystal.

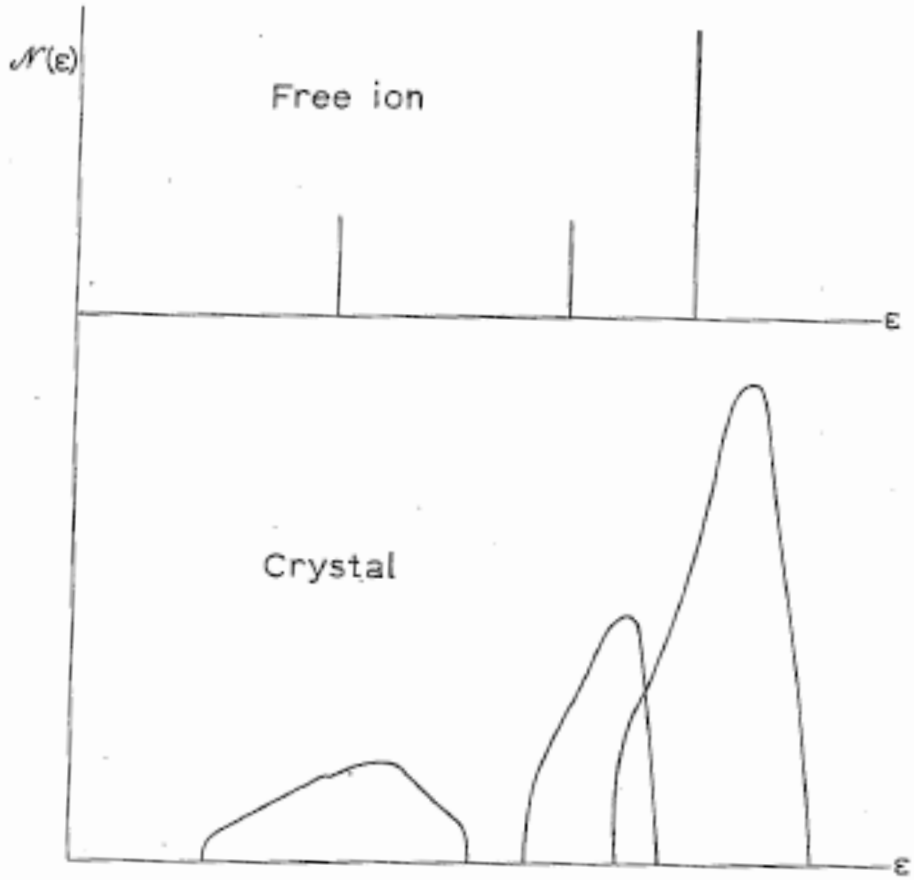


Fig. 4.2. Schematic density of states for electron in free ion (heights of lines proportional to degeneracy) and crystal, corresponding to fig. 4.1.

Some simple examples of band structure

CALCULATED

ELECTRONIC PROPERTIES

OF METALS

by

V. L. Moruzzi
J. F. Janak
A. R. Williams

IBM Thomas J. Watson Research Center
Yorktown Heights, New York

BM=-V (ΔP/ΔV)

$$(4/3)\pi r_s^3 = 1/\rho$$

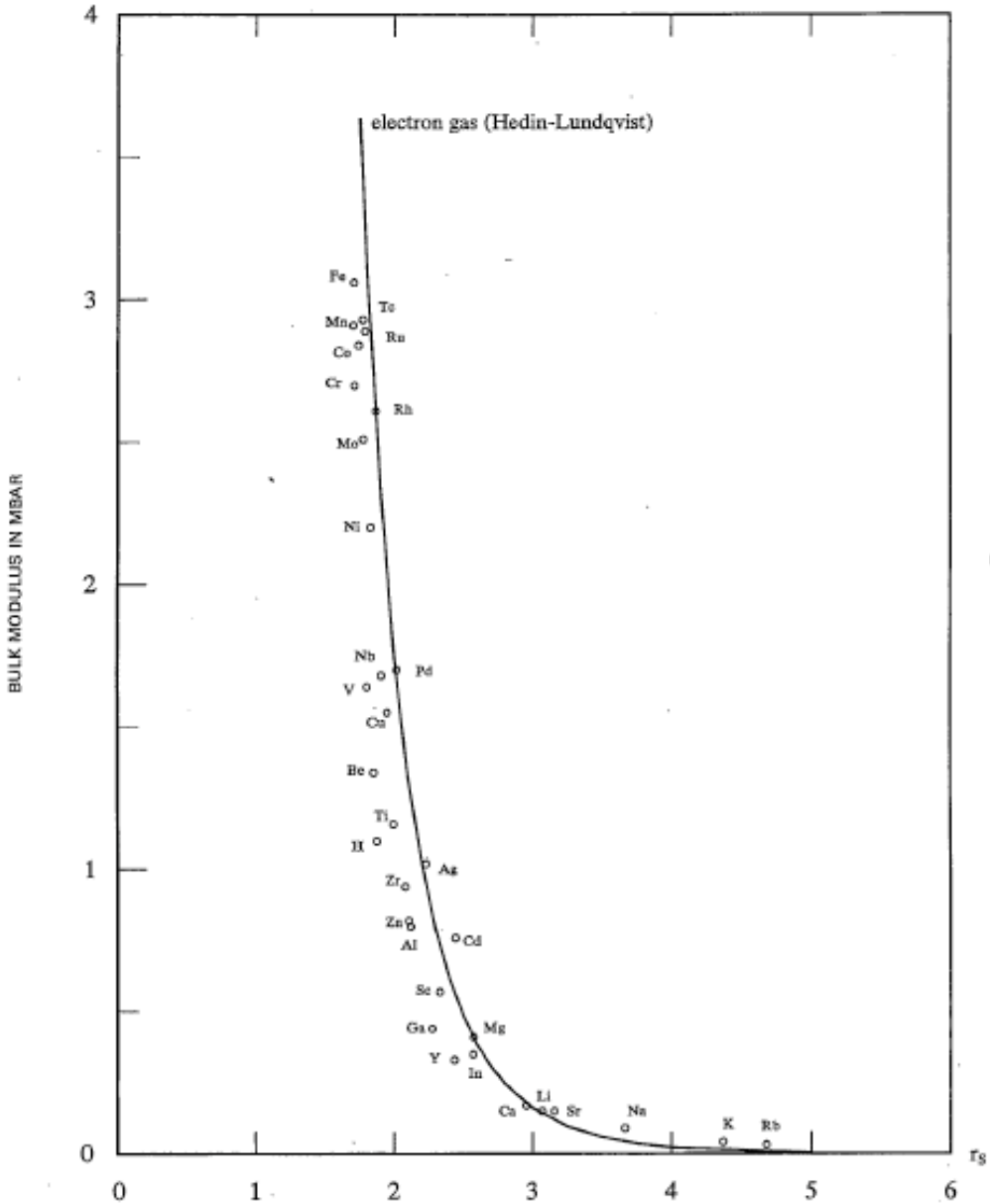


Figure 3.2 Bulk modulus vs r_s. The solid curve is the electron gas result. The points are the calculated bulk moduli (Mbar) at the r_s values derived from the interstitial charge density.

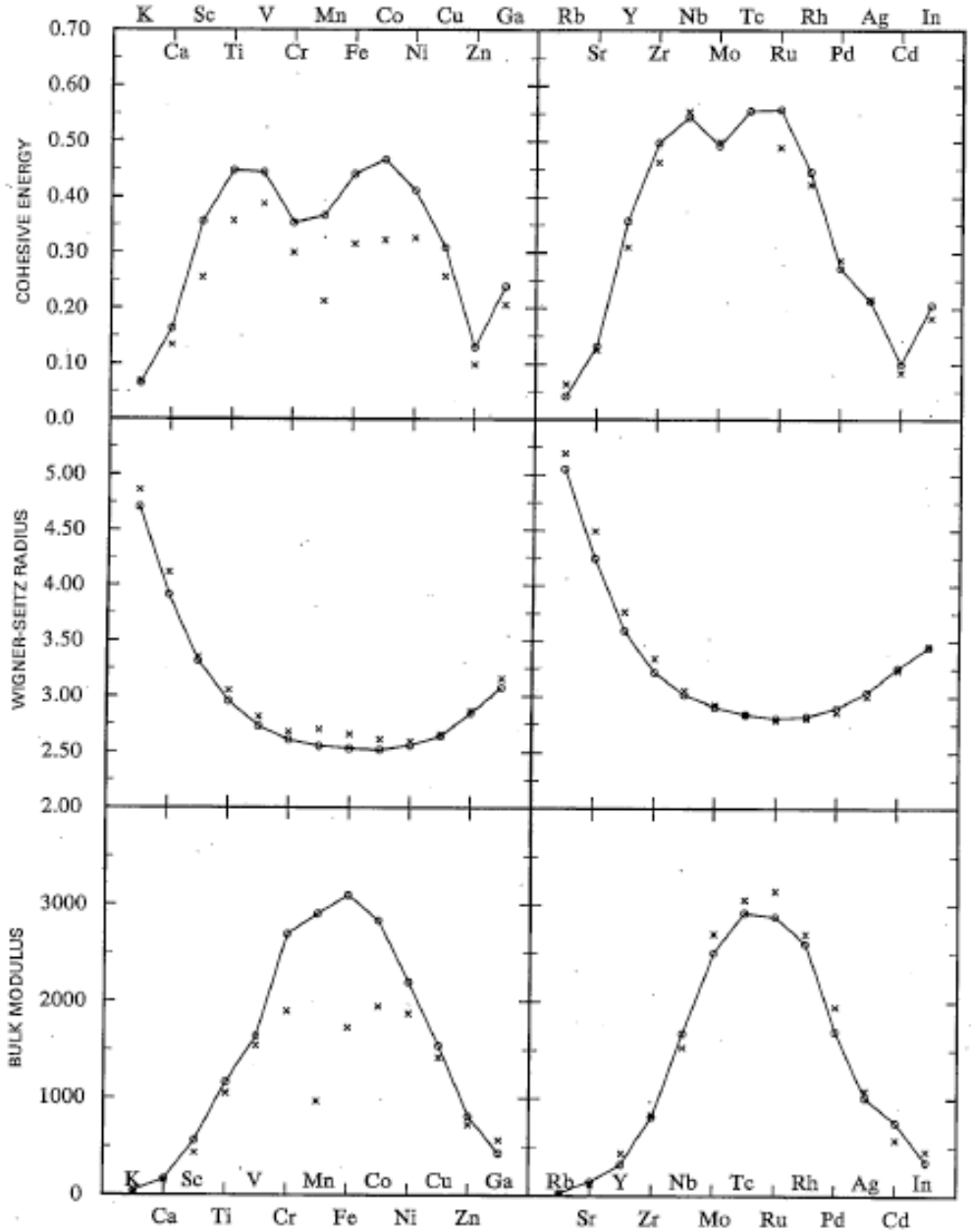
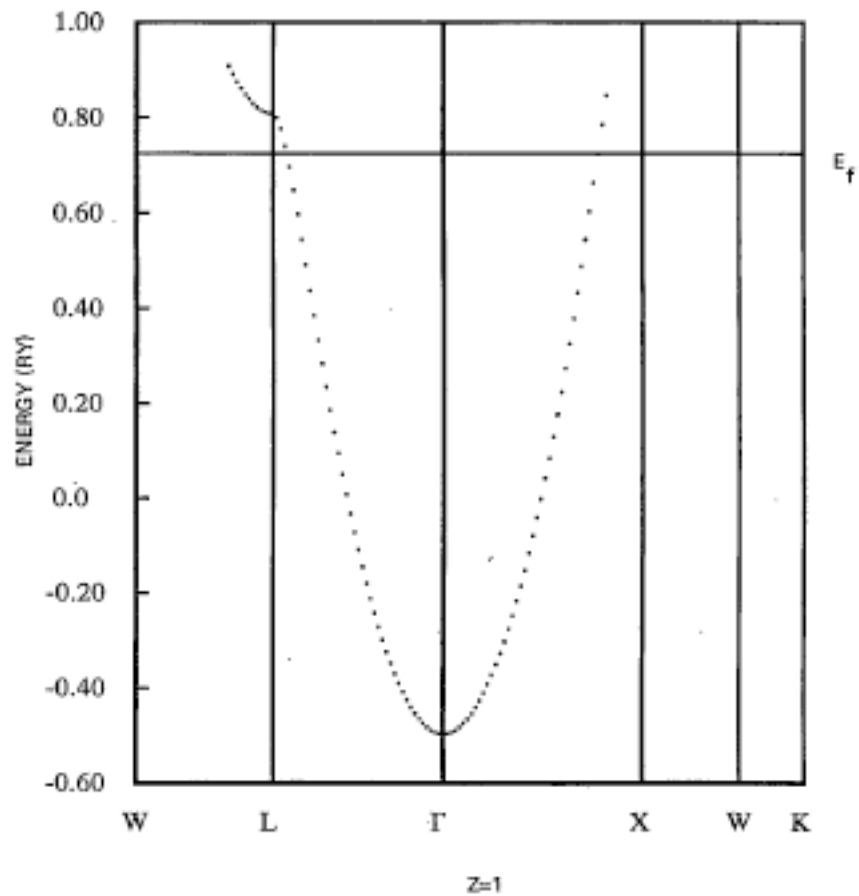


Figure 1.1 Cohesive properties. Top row- cohesive energy (Ry/atom). Middle row- Wigner-Seitz radius (a.u.). Bottom row- bulk modulus (Kbar). Measured values are indicated by crosses.

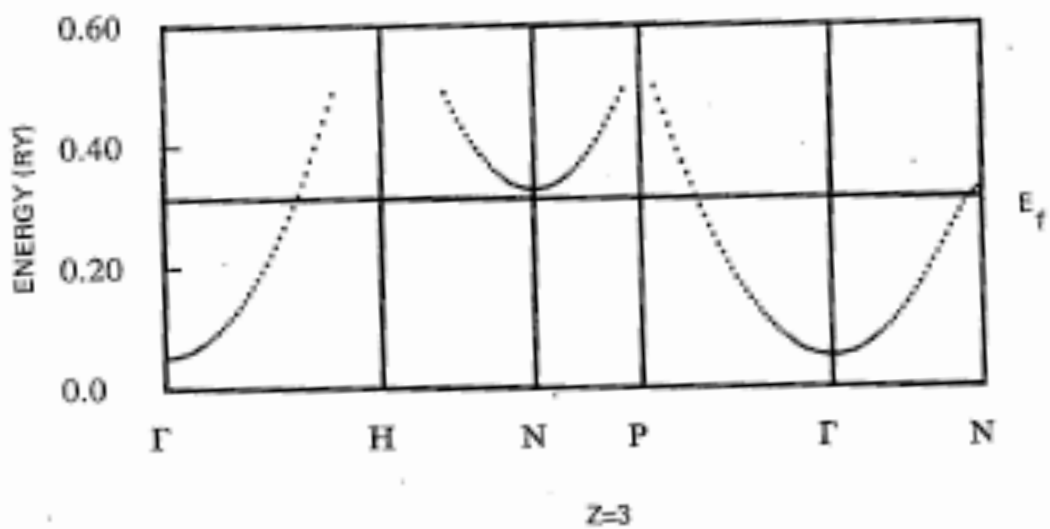
Hydrogen

Atomic Number	1
Lattice	fcc
Lattice constant a_o	4.30 a.u.
Pressure at a_o	6.9 Kbar
Total energy (solid)	-1.076 Ry
Total energy (atom)	-0.976 Ry
Zero point energy	0.000 Ry
Cohesive energy	0.100 Ry
Bulk modulus	1.10 Mbar
Fermi energy	0.724 Ry
Interstitial electrons (per atom)	0.187
χ/χ_o	1.40
$N(E_f)$	0.10 state
ρ_o	0.30 elect
$(d\rho(r,E)/dE)_{E=E_f,r=0}$	0.5120 ele



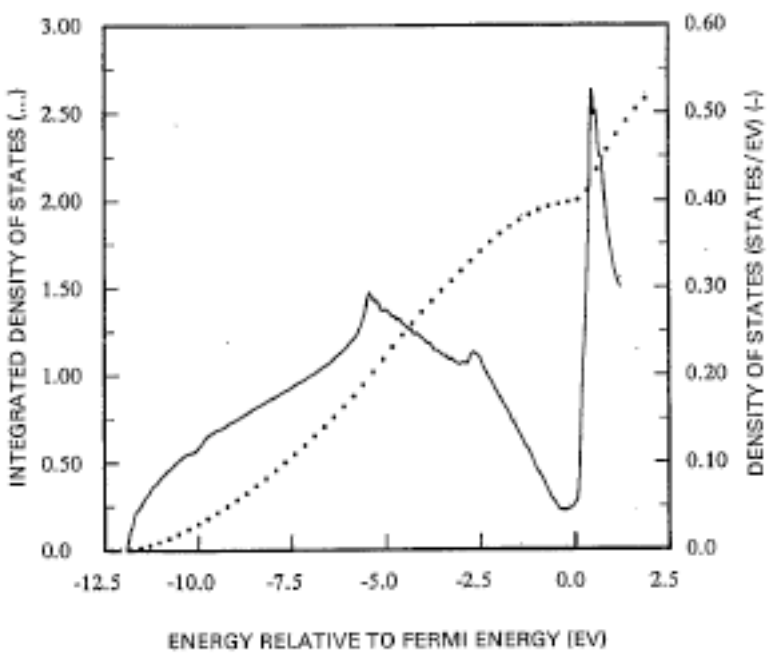
Lithium

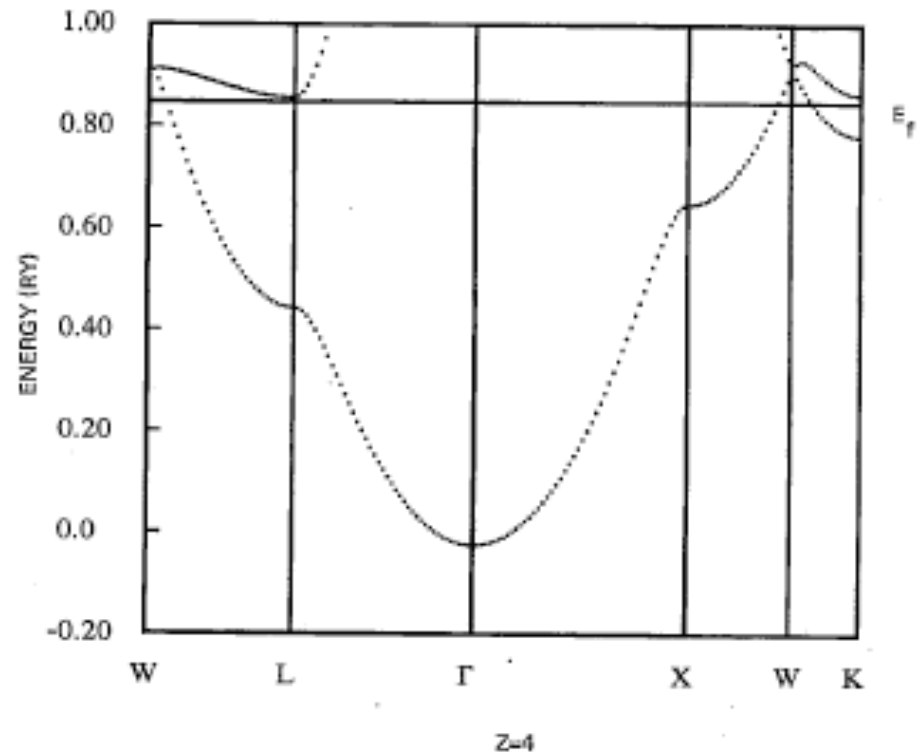
Atomic Number	3
Lattice	bcc
Lattice constant a_0	6.42 a.u.
Pressure at a_0	-1.06 Kbar
Total energy (solid)	-14.832 Ry
Total energy (atom)	-14.709 Ry
Zero point energy	0.003 Ry
Cohesive energy	0.121 Ry
Bulk modulus	0.15 Mbar
Fermi energy	0.313 Ry
Interstitial electrons (per atom)	0.350
χ/χ_0	2.25
$N(E_f)$	0.48 states/eV-atom
ρ_0	13.52 electrons/Bohr^3
$(d\rho(r,E)/dE)_{E=E_f,r=0}$	0.8638 electrons/Bohr^3-Ry



Beryllium

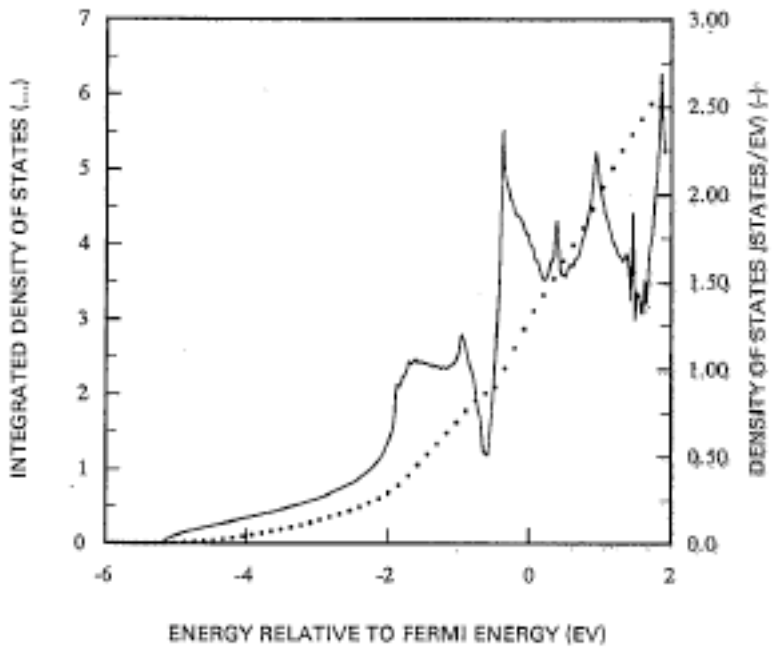
Atomic Number	4
Lattice	fcc
Lattice constant a_o	5.96 a.u.
Pressure at a_o	-22.5 Kbar
Total energy (solid)	-29.212 Ry
Total energy (atom)	-28.909 Ry
Zero point energy	0.011 Ry
Cohesive energy	0.292 Ry
Bulk modulus	1.34 Mbar
Fermi energy	0.845 Ry
Interstitial electrons (per atom)	0.516
χ/χ_o	1.06
$N(E_f)$	0.054 states/eV-atom
ρ_o	34.13 electrons/Bohr^3
$(d\rho(r,E)/dE)_{E=E_f,r=0}$	0.2560 electrons/Bohr^3-Ry

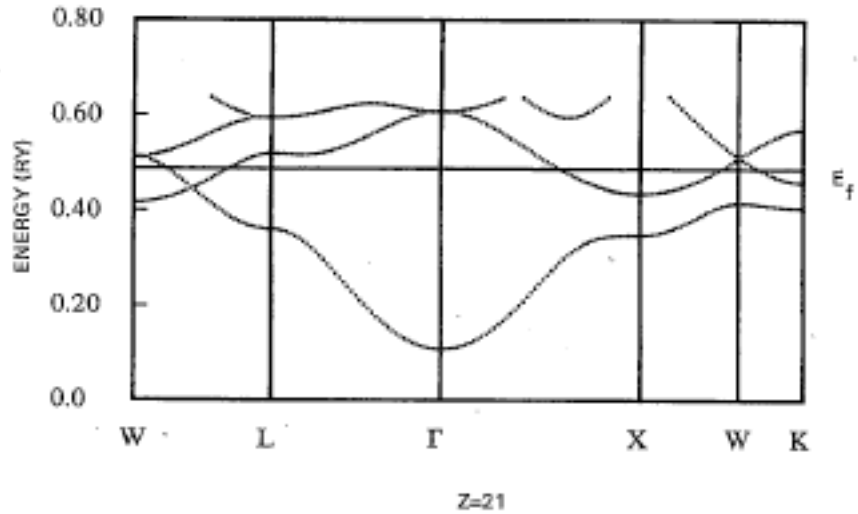




Scandium

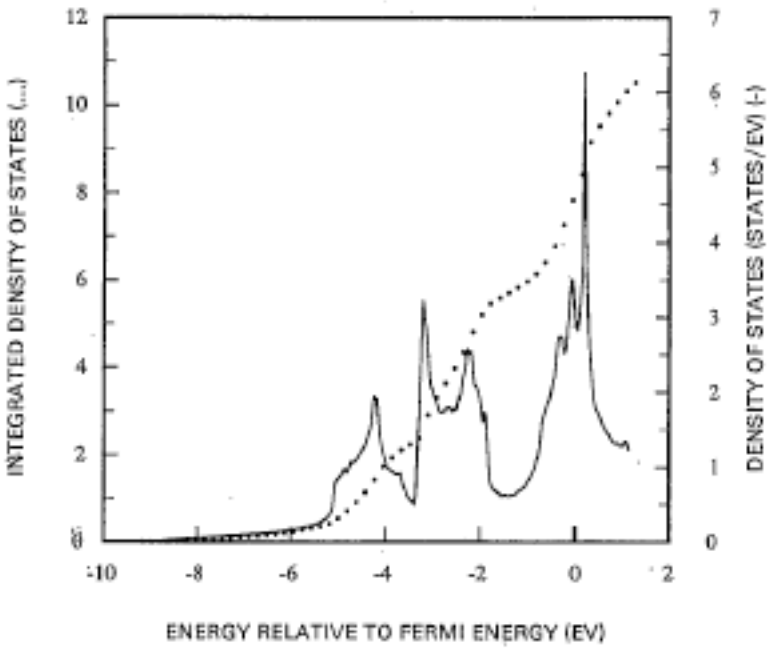
Atomic Number	21
Lattice	fcc
Lattice constant a_0	8.49 a.u.
Pressure at a_0	-8.3 Kbar
Total energy (solid)	-1517.685 Ry
Total energy (atom)	-1517.322 Ry
Zero point energy	0.003 Ry
Cohesive energy	0.360 Ry
Bulk modulus	0.57 Mbar
Fermi energy	0.488 Ry
Interstitial electrons (per atom)	0.748
χ/χ_0	2.47
$N(E_f)$	1.73 states/eV-atom
ρ_0	6.152×10^3 electrons/Bohr^3
$(d\rho(r,E)/dE)_{E=E_f,r=0}$	3.0394 electrons/Bohr^3-Ry

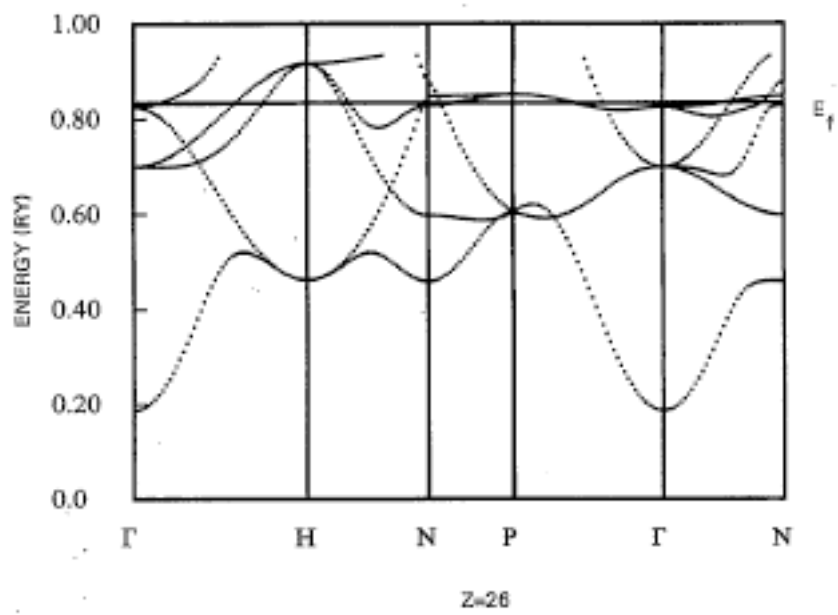




Iron

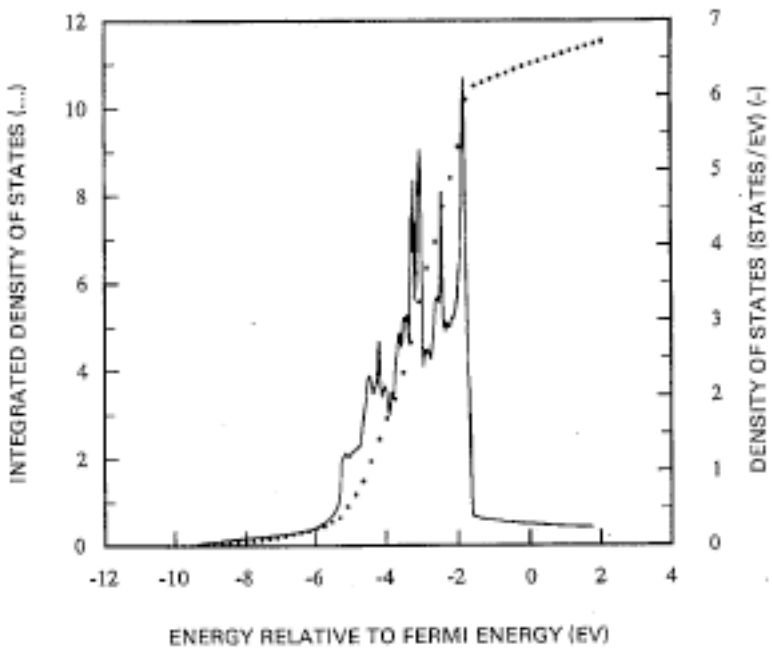
Atomic Number	26
Lattice	bcc
Lattice constant a_0	5.15 a.u.
Pressure at a_0	-8.28 Kbar
Total energy (solid)	-2522.812 Ry
Total energy (atom)	-2522.369 Ry - see p. 168
Zero point energy	0.004 Ry
Cohesive energy	0.439 Ry
Bulk modulus	3.06 Mbar
Fermi energy	0.833 Ry
Interstitial electrons (per atom)	1.044
χ/χ_0	-2.34
$N(E_f)$	3.06 states/eV-atom
ρ_0	1.186×10^4 electrons/Bohr^3
$(d\rho(r,E)/dE)_{E=E_f,r=0}$	1.9133 electrons/Bohr^3-Ry

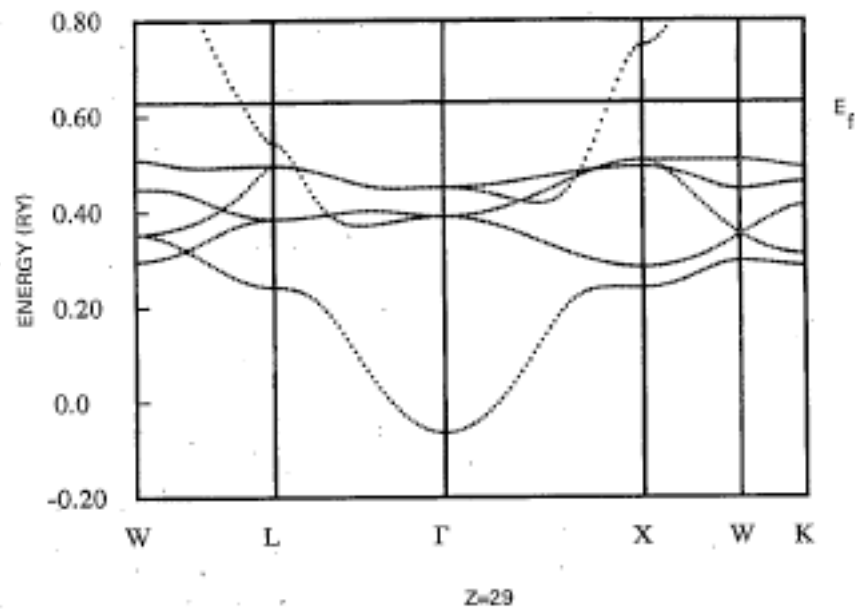




Copper

Atomic Number	29
Lattice	fcc
Lattice constant a_0	6.76 a.u.
Pressure at a_0	4.94 Kbar
Total energy (solid)	-3275.768 Ry
Total energy (atom)	-3275.464 Ry
Zero point energy	0.003 Ry
Cohesive energy	0.301 Ry
Bulk modulus	1.55 Mbar
Fermi energy	0.628 Ry
Interstitial electrons (per atom)	0.647
χ/χ_0	1.12
$N(E_f)$	0.29 states/eV-atom
ρ_0	1.657×10^4 electrons/Bohr^3
$(d\rho(r,E)/dE)_{E=E_f,r=0}$	6.2372 electrons/Bohr^3-Ry





Phonons, Energy Landscapes, and Electronic Structure

ICOMAT

Bruce Harmon

Iowa State University
And
Ames Laboratory

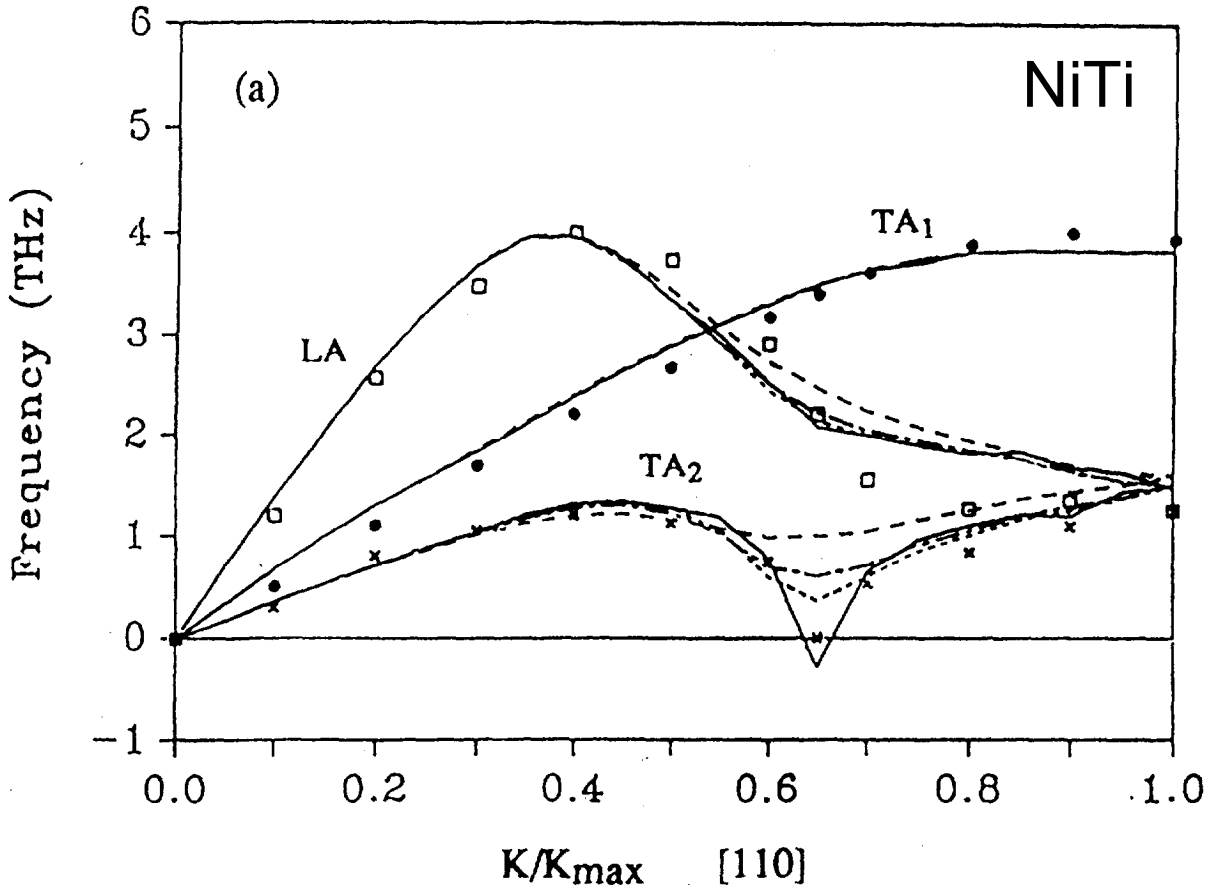
Outline

Soft phonon modes association
with some
Martensitic Transformations

Energy Landscapes

Dynamics

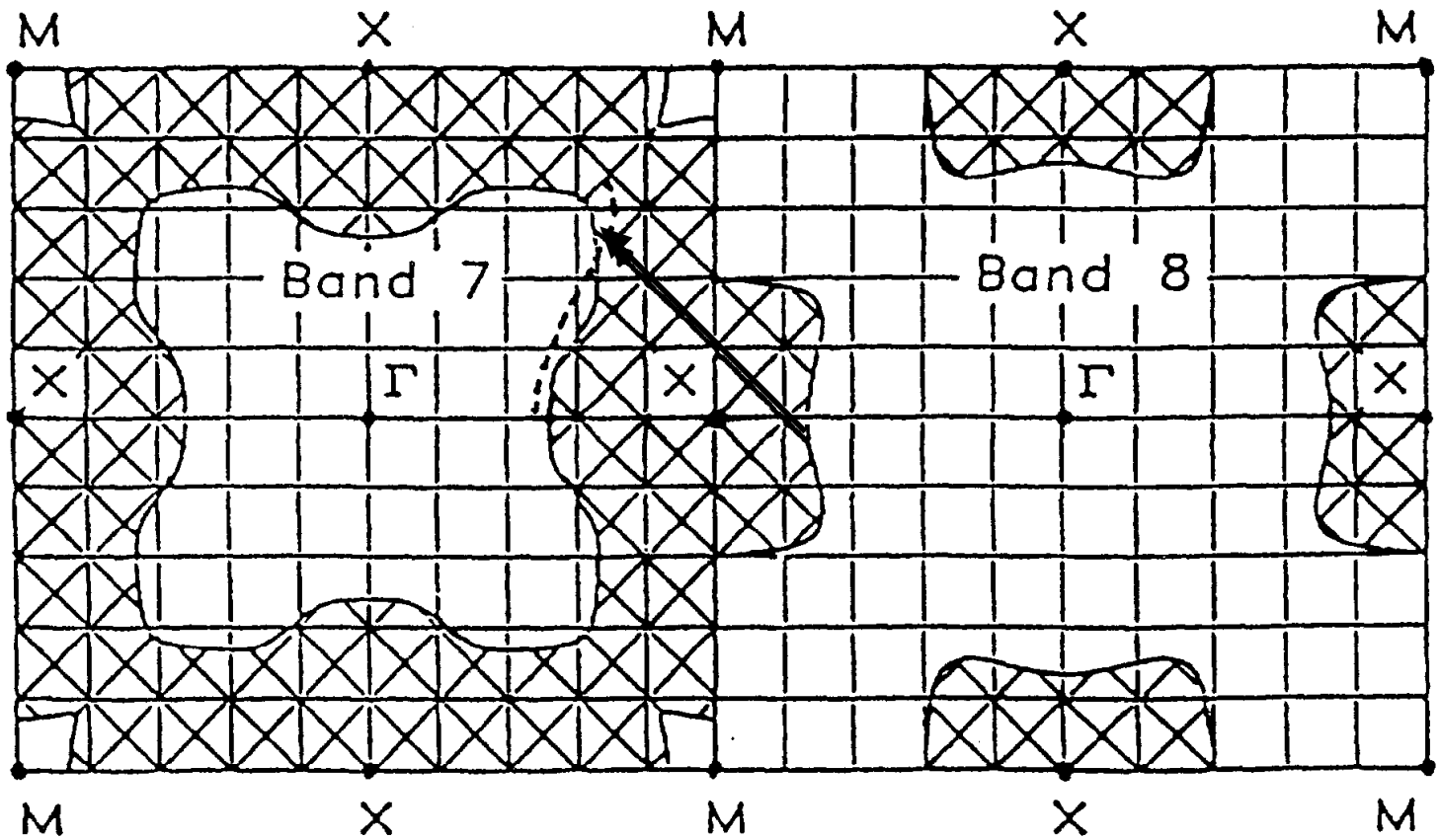
Magnetic Influences



T = 0 K
320 K
500 K
1000 K

Theory - G.L. Zhao and B.N.Harmon, Phys. Rev. B48, 2031 (1993)

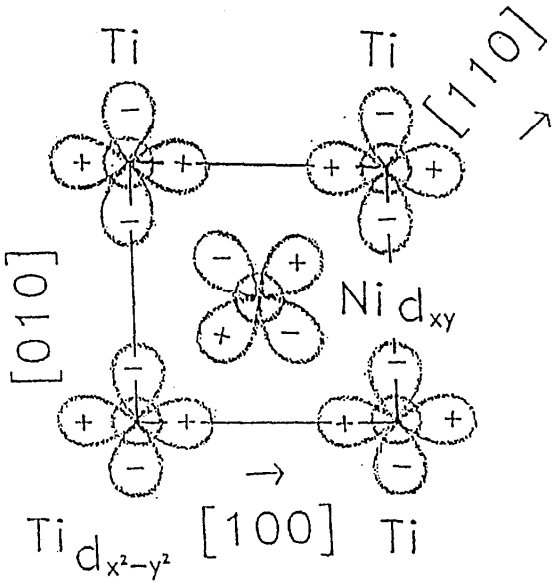
Experiment - H. Tietz, M. Müllner, and B Renker, J. Phys. F 14, 2517 (1984)


M
X
M
X
M
Band 7
Band 8
X
Γ
X
Γ
X
M
X
M
X
M

Dynamical Matrix -

Conduction electrons

$$D_2(\kappa\alpha,\kappa'\alpha'|\mathbf{q}) = -\sum_{\mathbf{k}\mu\nu} \frac{f_{\mathbf{k}\mu}(1-f_{\mathbf{k}+\mathbf{q}\nu})}{\varepsilon_{\mathbf{k}+\mathbf{q}\nu}-\varepsilon_{\mathbf{k}\mu}} \times g^{\kappa\alpha}_{\mathbf{k}\mu,\mathbf{k}+\mathbf{q}\nu} g^{\kappa'\alpha'}_{\mathbf{k}+\mathbf{q}\nu,\mathbf{k}\mu} ,$$



Importance of el-ph

Matrix elements