Some interesting materials

There is no video for this lecture. I forgot to press ‘record’ at the beginning of the lecture.

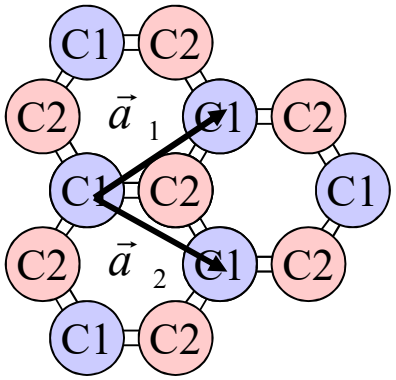
Exam

One A4 handwritten notes
One hour
Like the exams online

polytypes

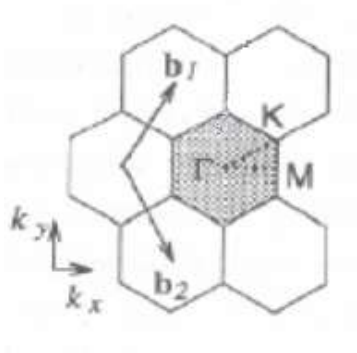
Different polytypes ⇨ Different properties

Graphene



$$\vec{a}_1 = \frac{\sqrt{3}}{2} a\hat{x} + \frac{1}{2} a\hat{y}$$

$$\vec{a}_2 = \frac{\sqrt{3}}{2} a\hat{x} - \frac{1}{2} a\hat{y}$$

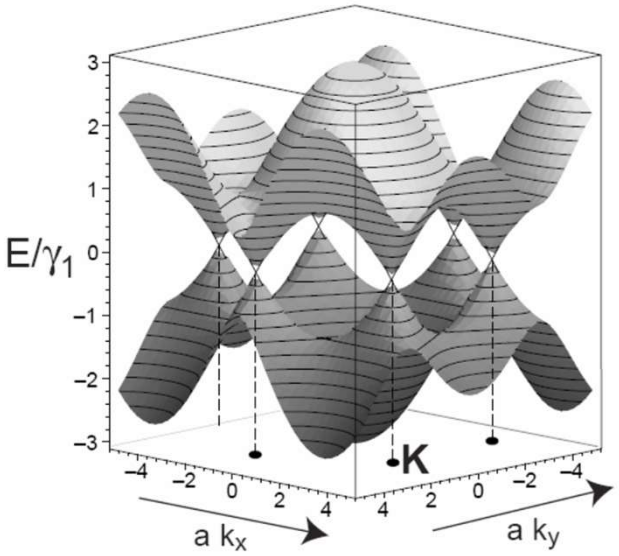


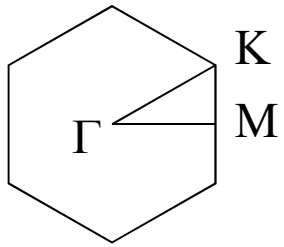
Two atoms per unit cell

Graphene has an unusual dispersion relation in the vicinity of the Fermi energy.

Tight binding, graphene

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$



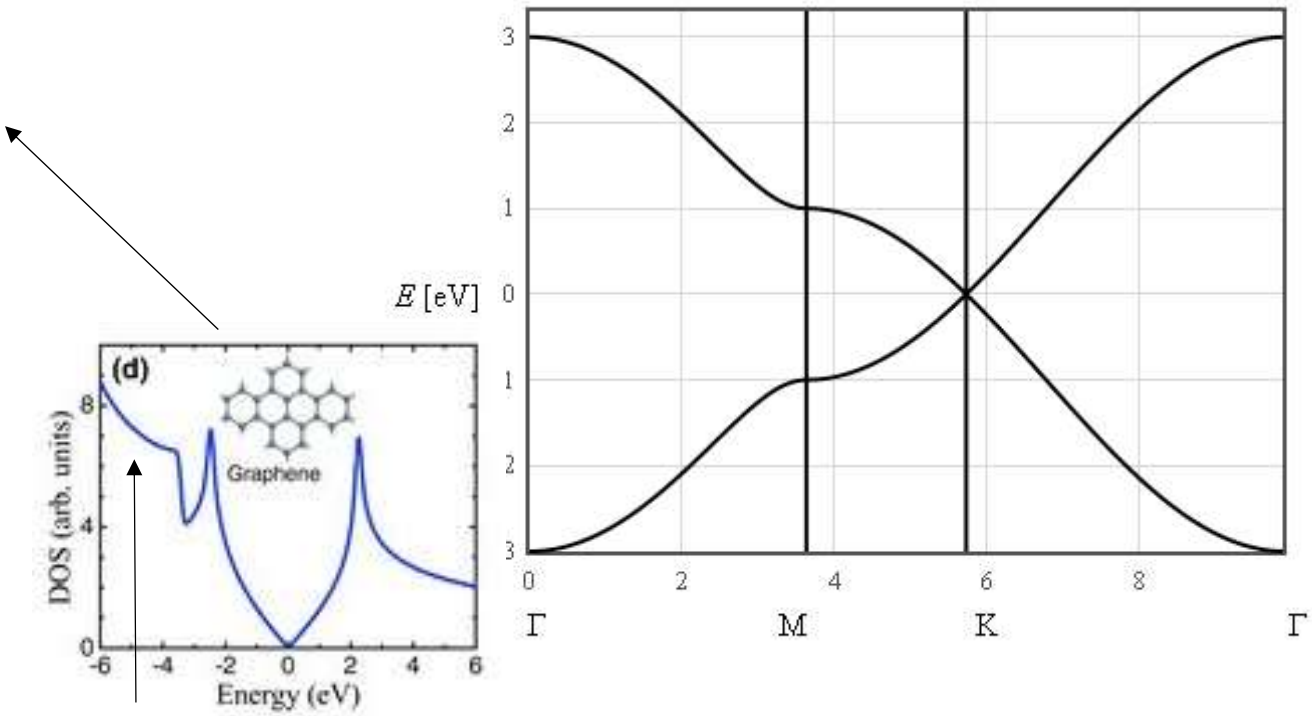


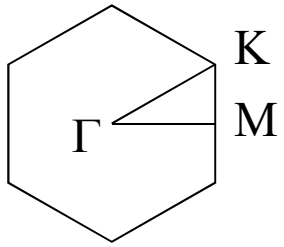
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

http://onlinelibrary.wiley.com/doi/10.1002/adfm.201101241/full

Tight binding dispersion relation for graphene

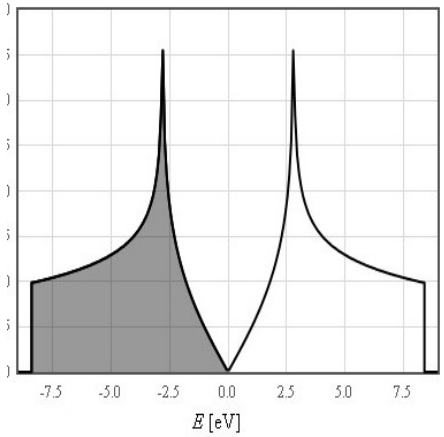
$$E = \varepsilon \pm t\sqrt{1+4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_y a}{2}\right)}$$





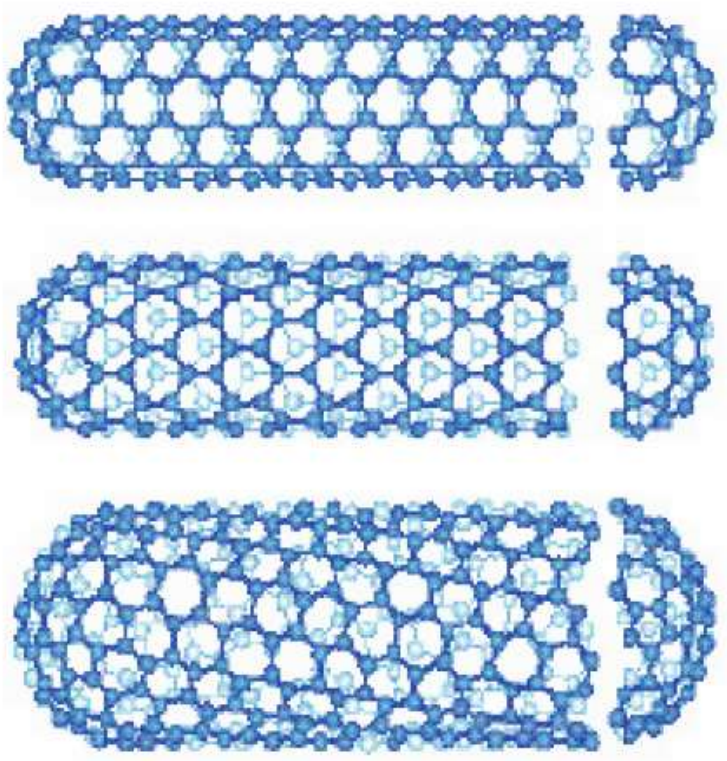
ε = 0 [eV]
t = 2.8 [eV]
Replot E(k)

Another band is included here.



http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/dispgraphene.html

Carbon nanotubes - rolled up graphene



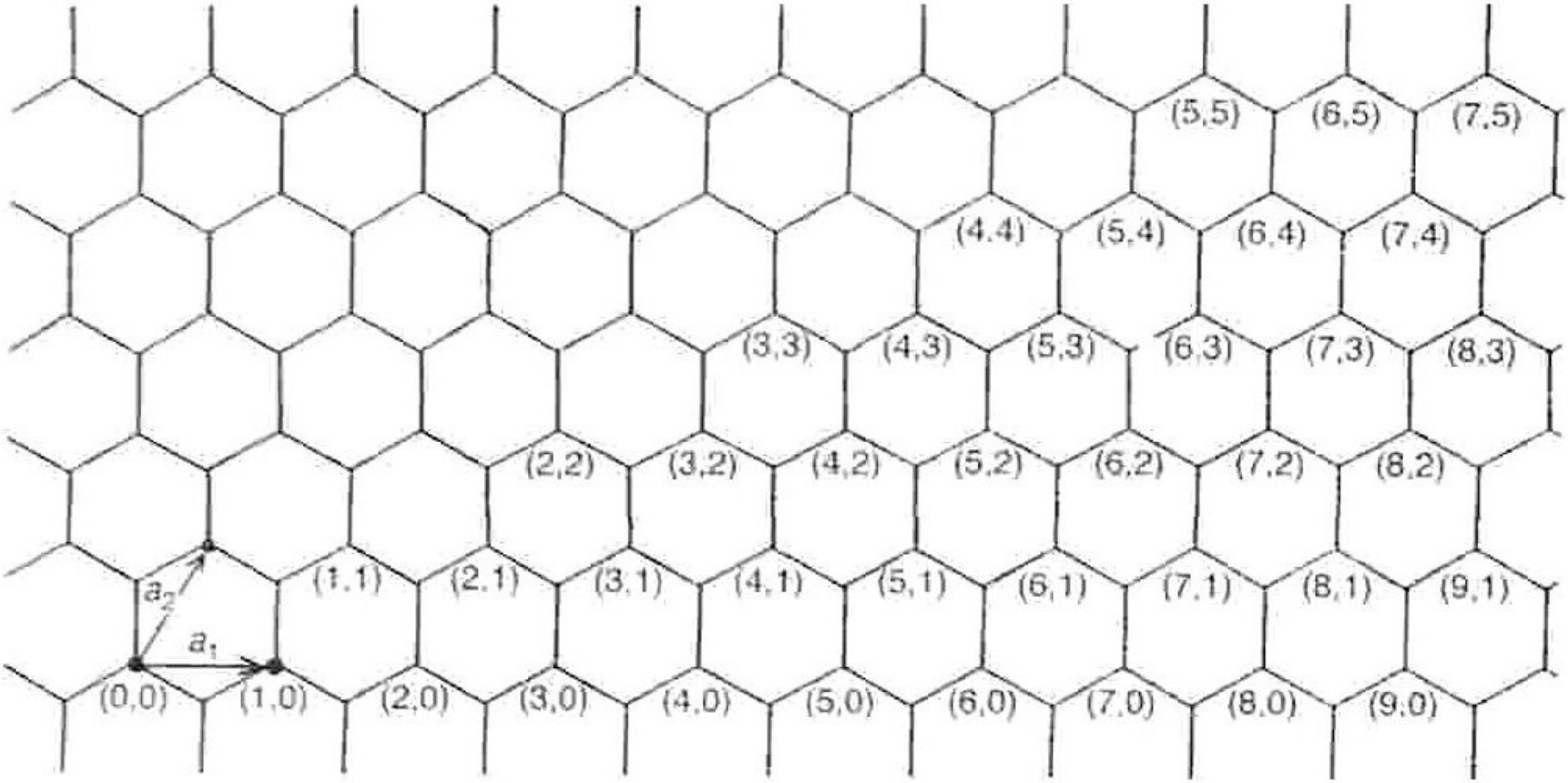
armchair

zig-zag

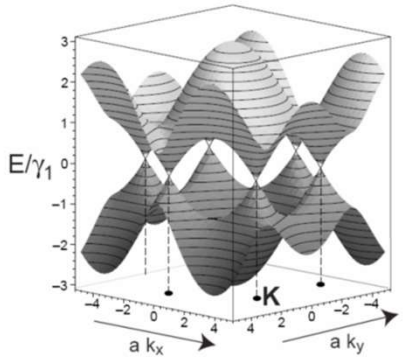
chiral

www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

(*m*,*n*) notation

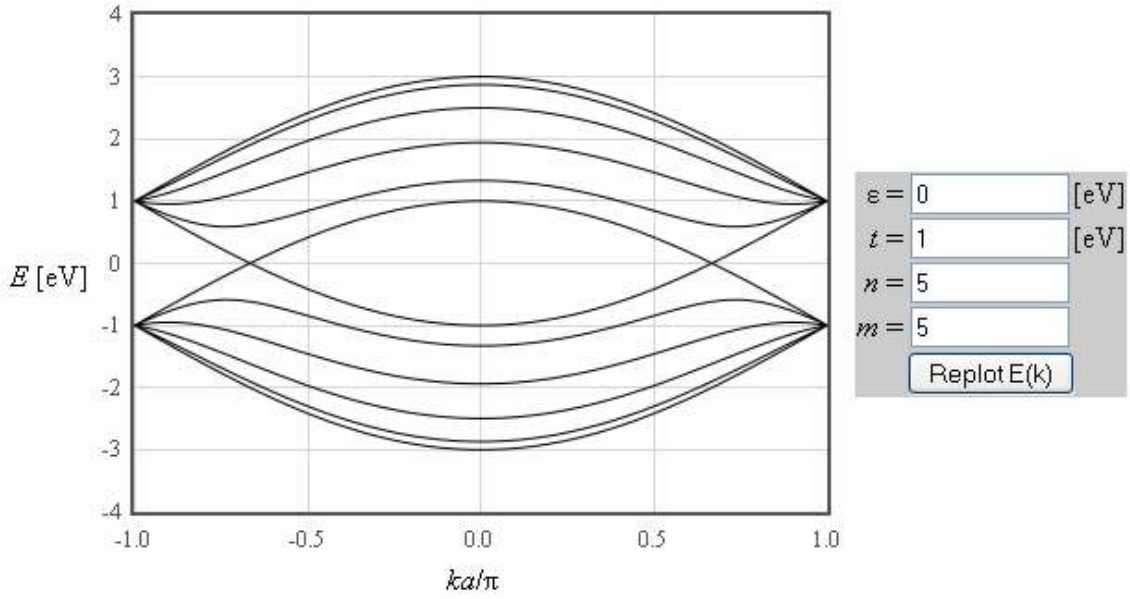


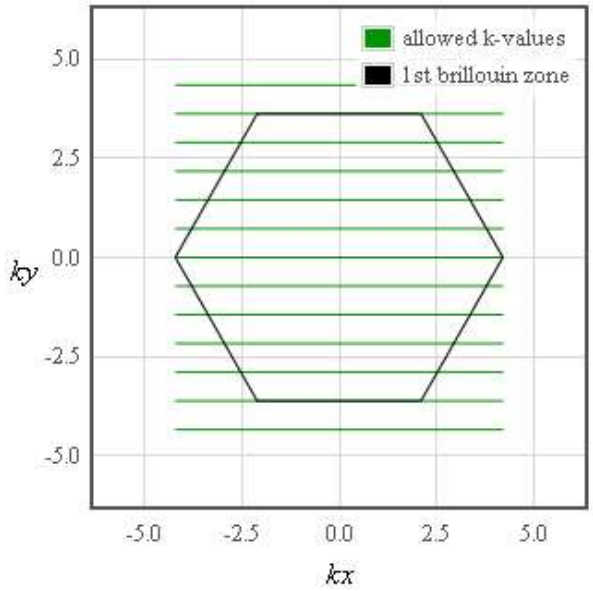
http://www.personal.rdg.ac.uk/~scsharip/tubes.htm



Carbon nanotubes

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$

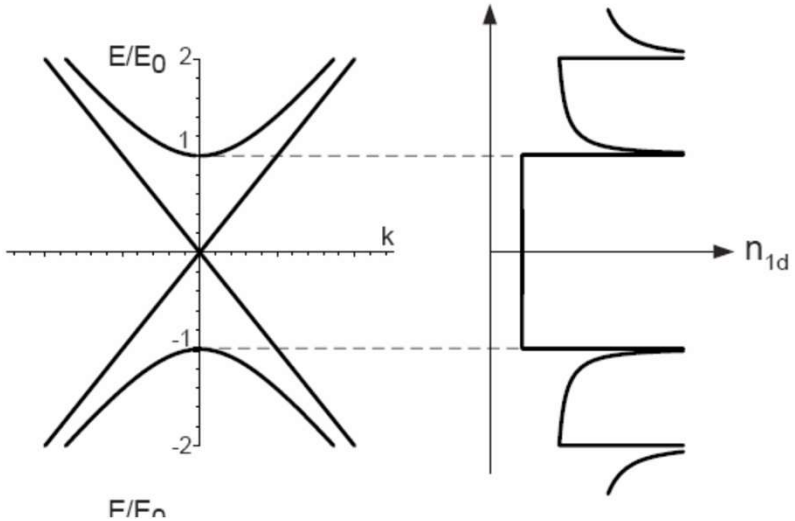


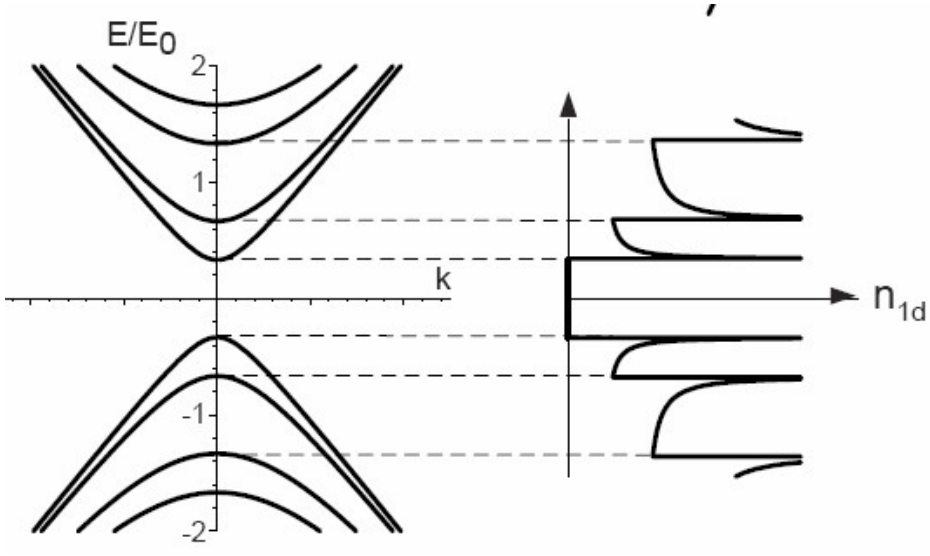


metallic (5,5) armchair tube

http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/CNTs.html

Carbon nanotubes

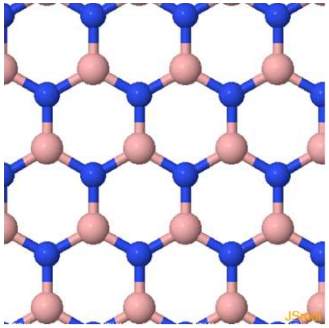




metallic $m - n = 3Z$

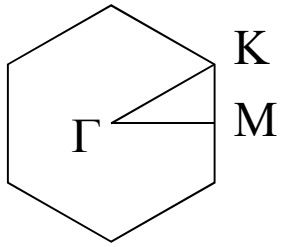
semiconducting

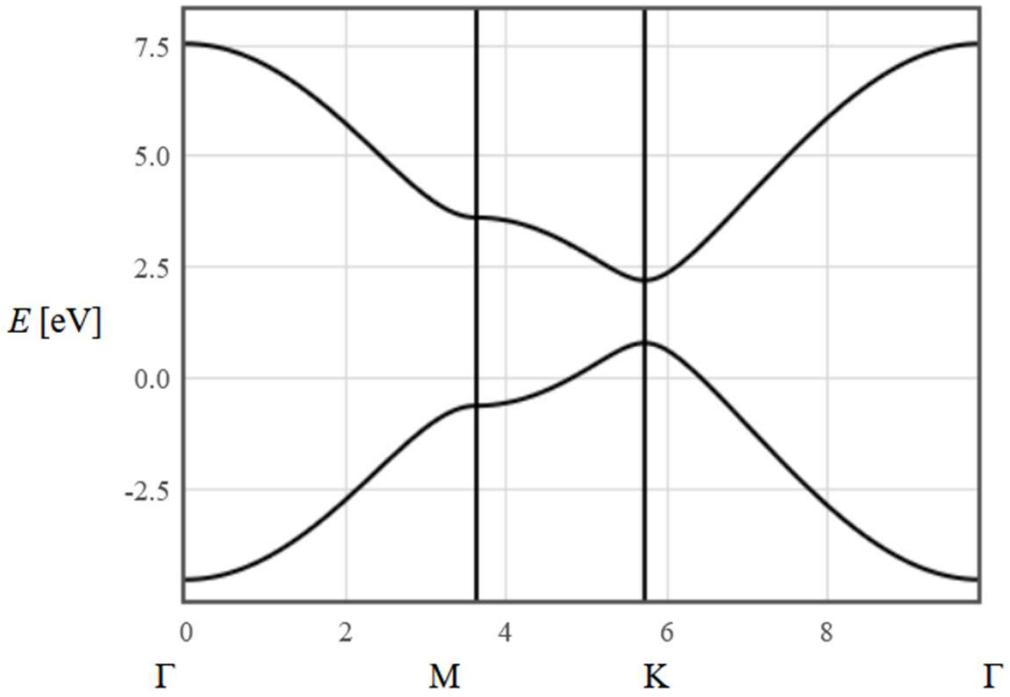
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

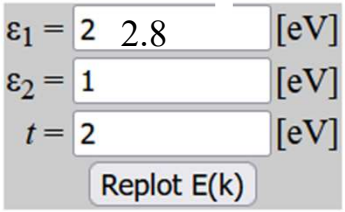


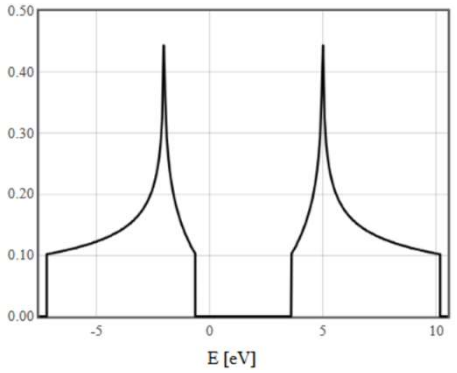
2-D boron nitride

$$E = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \sqrt{\frac{(\varepsilon_1 - \varepsilon_2)^2}{2} + 4t^2\left(\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos^2\left(\frac{k_y a}{2}\right) + \frac{1}{4}\right)}$$



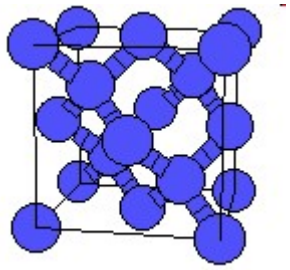




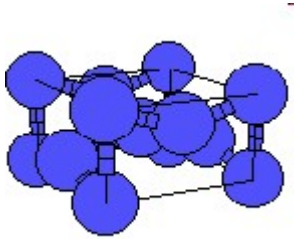


http://lampz.tugraz.at/~hadley/ss1/bands/tbtable/dispbn.html

Structural phase transitions

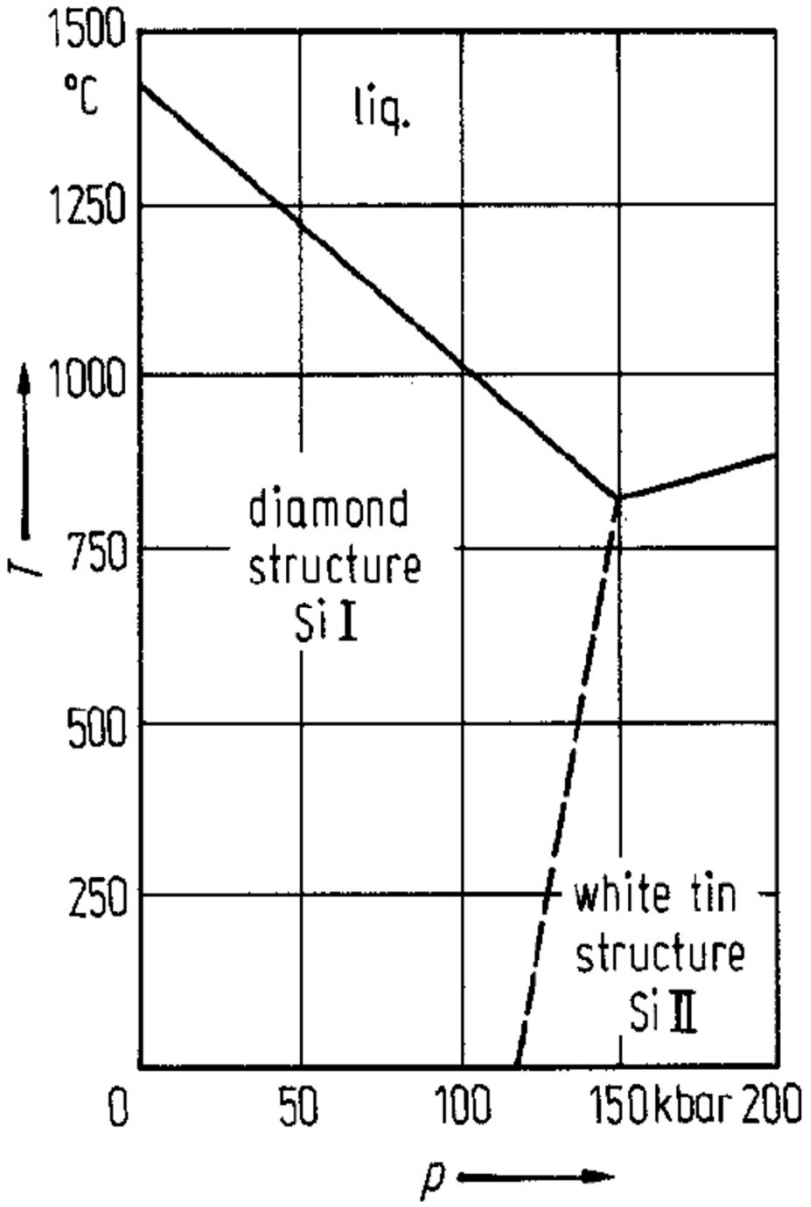


Si, diamond structure

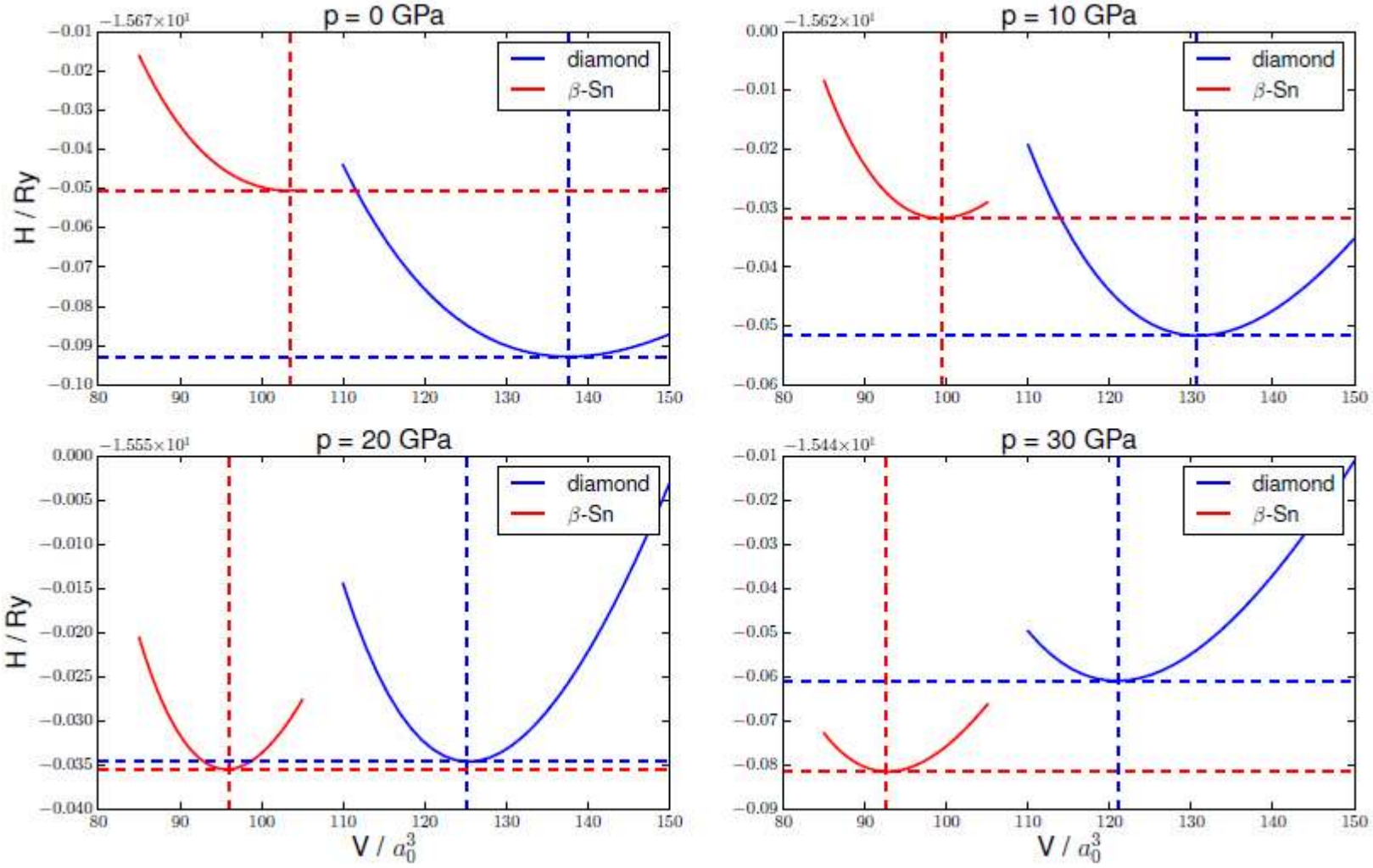


Si II, β-Sn, tetragonal

silicon makes a diamond to β-Sn transition under pressure



Structural phase transition in Si



Michael Scherbela 2015

Structural phase transition in Si

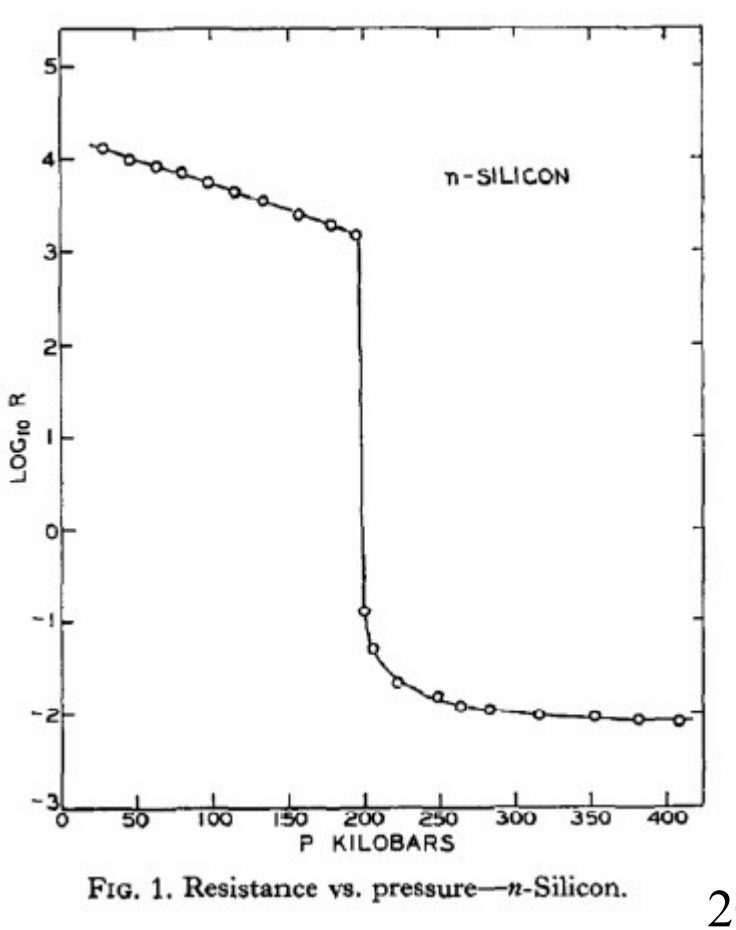
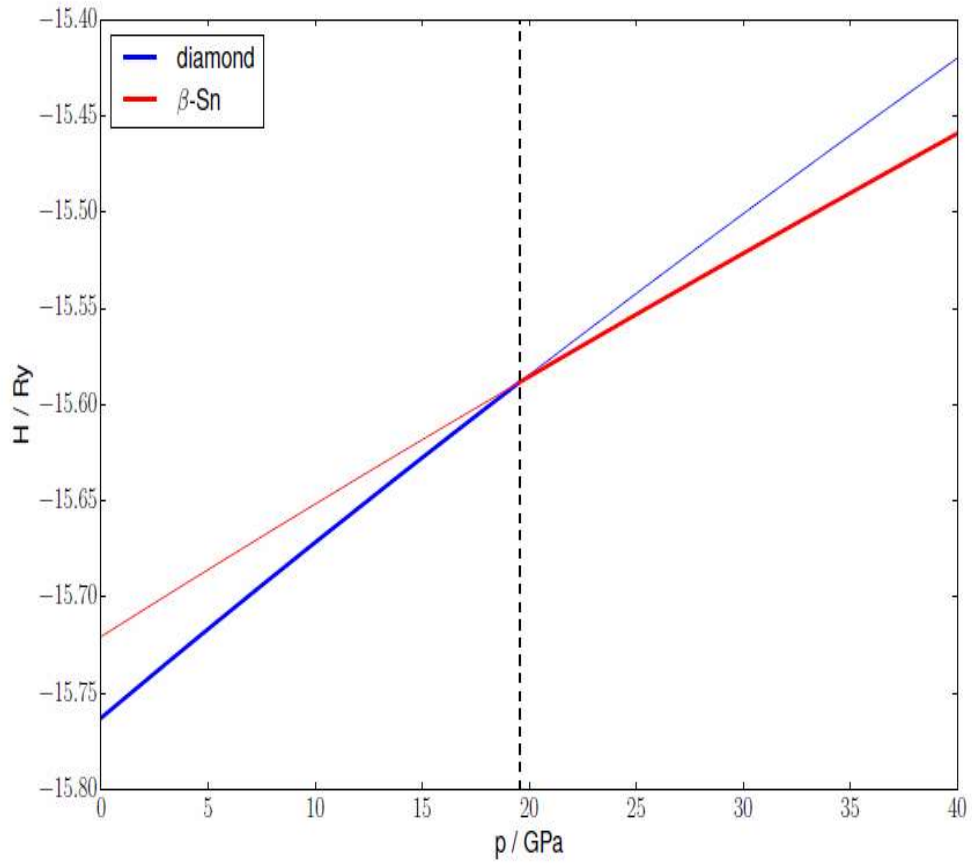


FIG. 1. Resistance vs. pressure—*n*-Silicon.



200 kbar = 20 GPa

Michael Scherbela 2015

H. G. D. S. Minomura, "Pressure induced phase transitions in silicon, germanium and some iii-v compounds," *J. Phys. Chem. Solids Pergamon Press*, vol. 23, pp. 451–456, 1962.

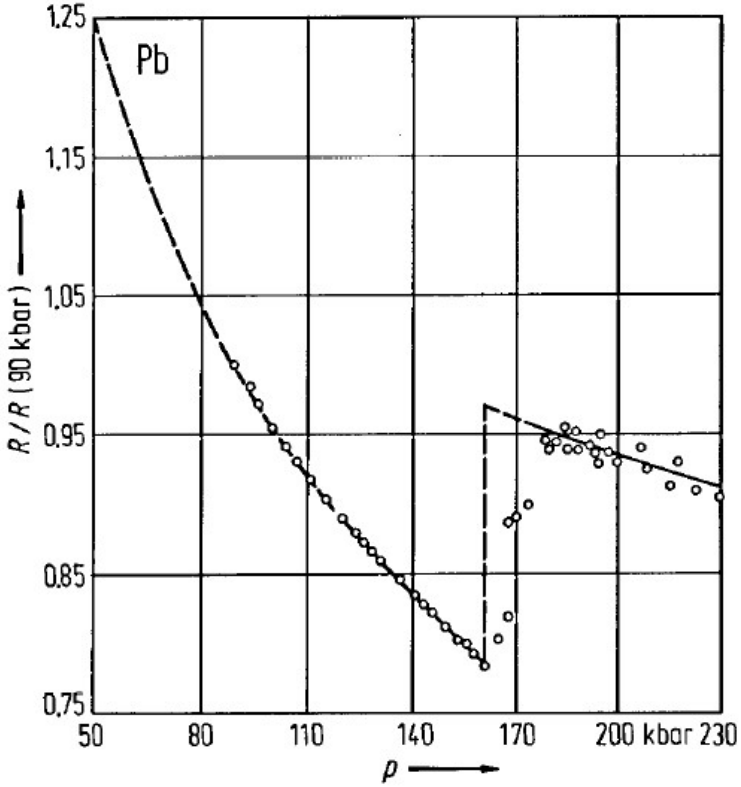
Strain

Strain displaces the atoms and the band structure needs to be recalculated.

This changes the density of states and the thermodynamic properties.

Make Legendre transformations from the internal energy to the enthalpy that has temperature and pressure as independent variables. The crystal structure with lowest enthalpy will be observed.

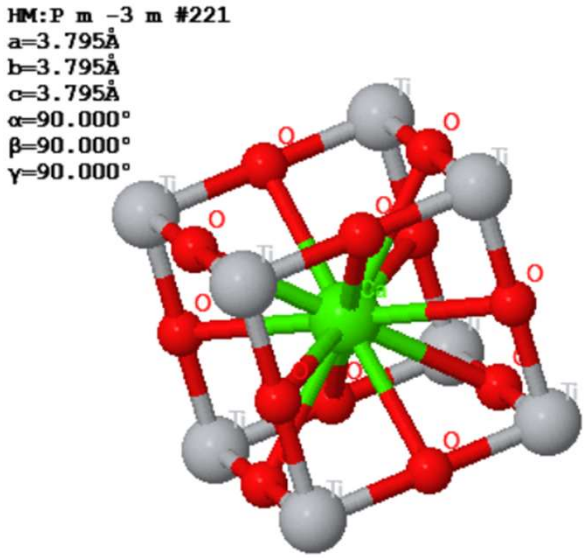
Enthalpy is calculated from the microscopic states of electrons and phonons.



Ferroelectricity

ABX_3

Perovskites

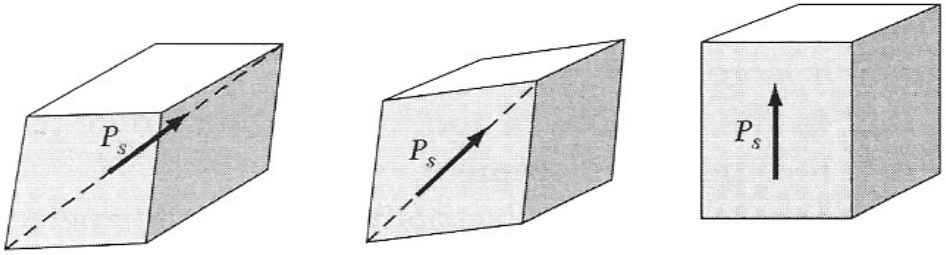


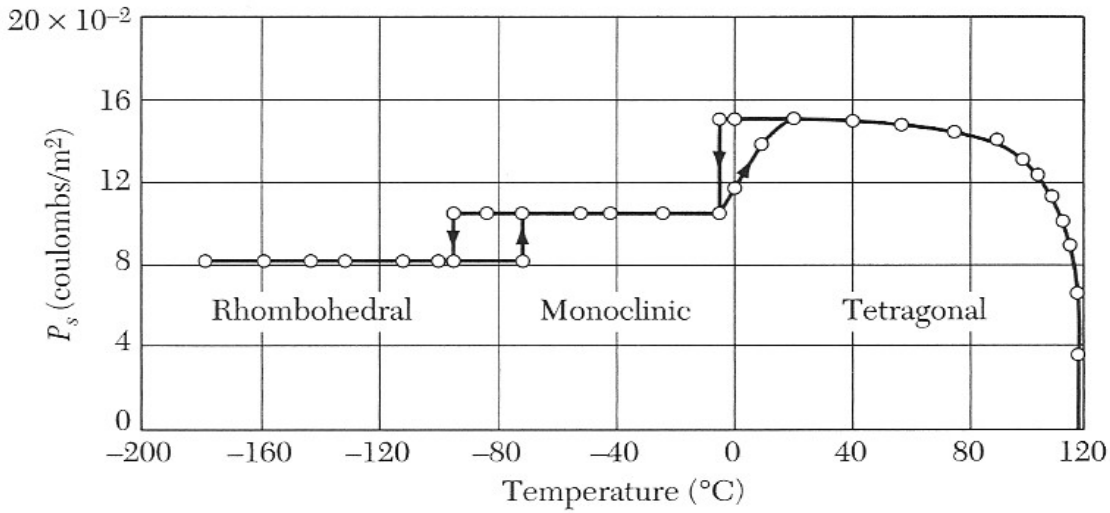
Spontaneous polarization
Analogous to ferromagnetism
Structural phase transition
T_c is transition temperature

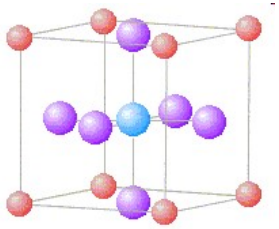
Electric field inside the material, is not conducting

		T_c, in K	P_s, in μC cm^{-2}, at T K	
KDP type	KH_2PO_4	123	4.75	[96]
	KD_2PO_4	213	4.83	[180]
	RbH_2PO_4	147	5.6	[90]
	KH_2AsO_4	97	5.0	[78]
	GeTe	670	—	—
TGS type	Tri-glycine sulfate	322	2.8	[29]
	Tri-glycine selenate	295	3.2	[283]
Perovskites	$BaTiO_3$	408	26.0	[296]
	$KNbO_3$	708	30.0	[523]
	$PbTiO_3$	765	>50	[296]
	$LiTaO_3$	938	50	
	$LiNbO_3$	1480	71	[296]

$BaTiO_3$

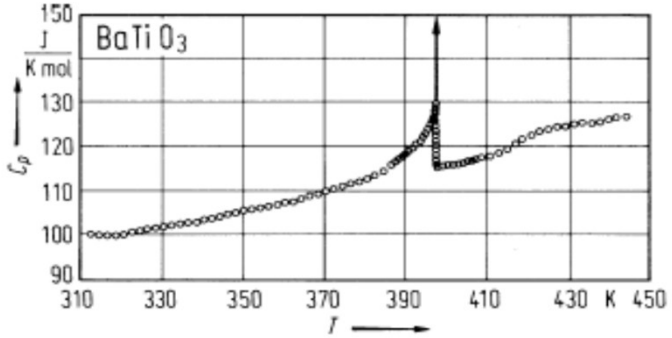






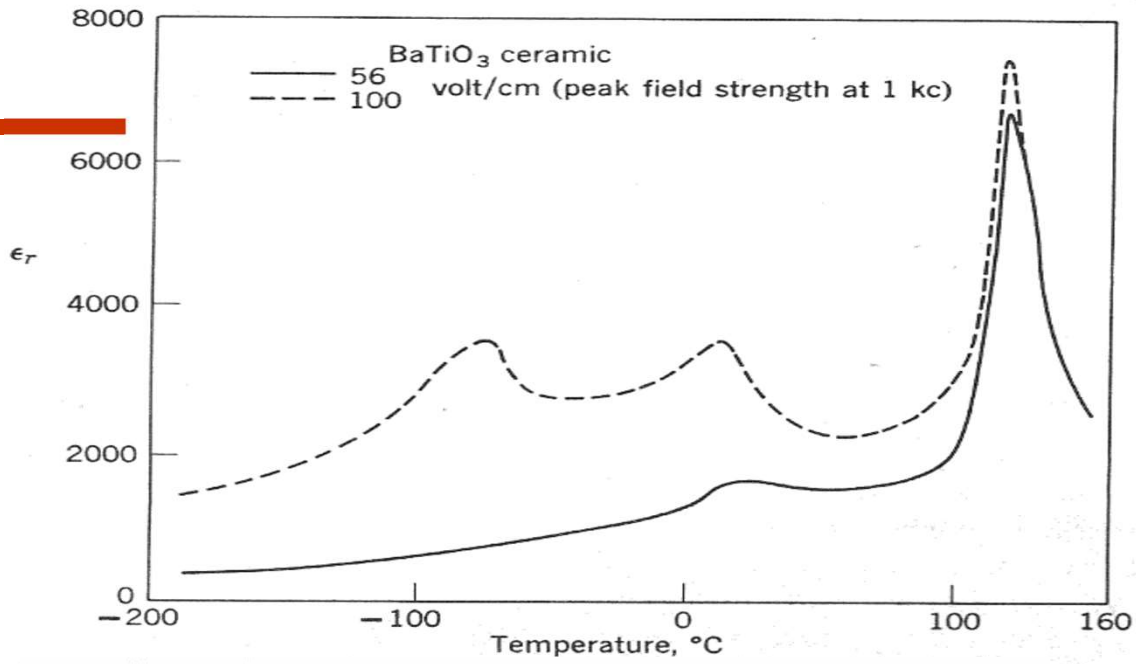
cubic (contains i = > no spontaneous P)

Can be used to make nonvolatile memory

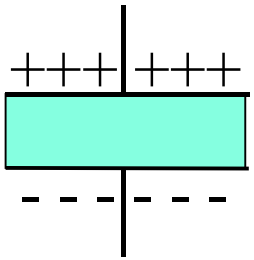


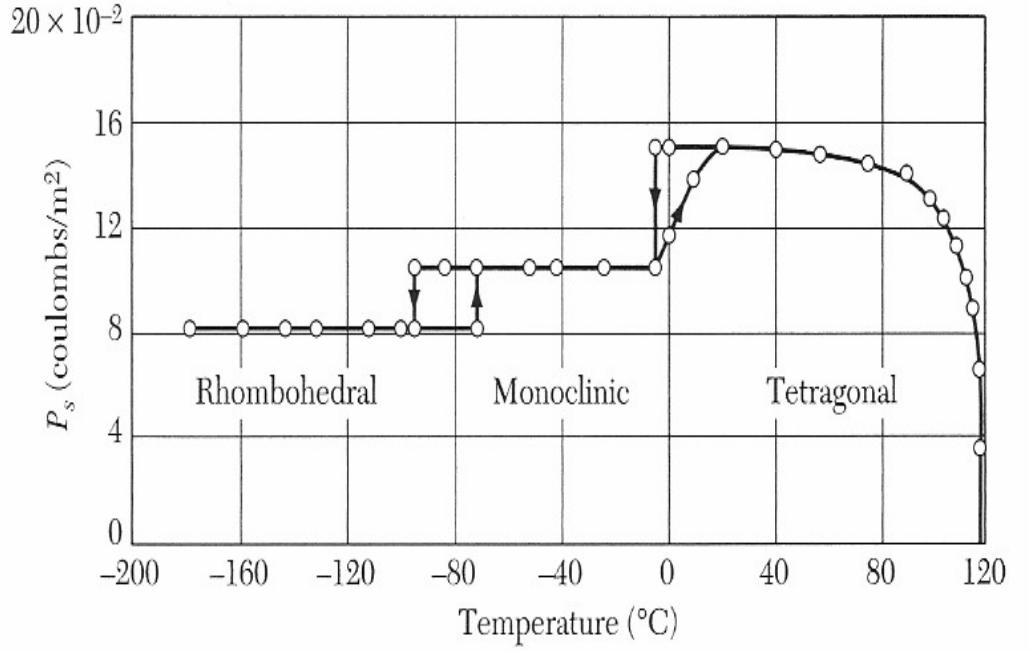
$BaTiO_3$

$$\varepsilon_r = \chi + 1$$

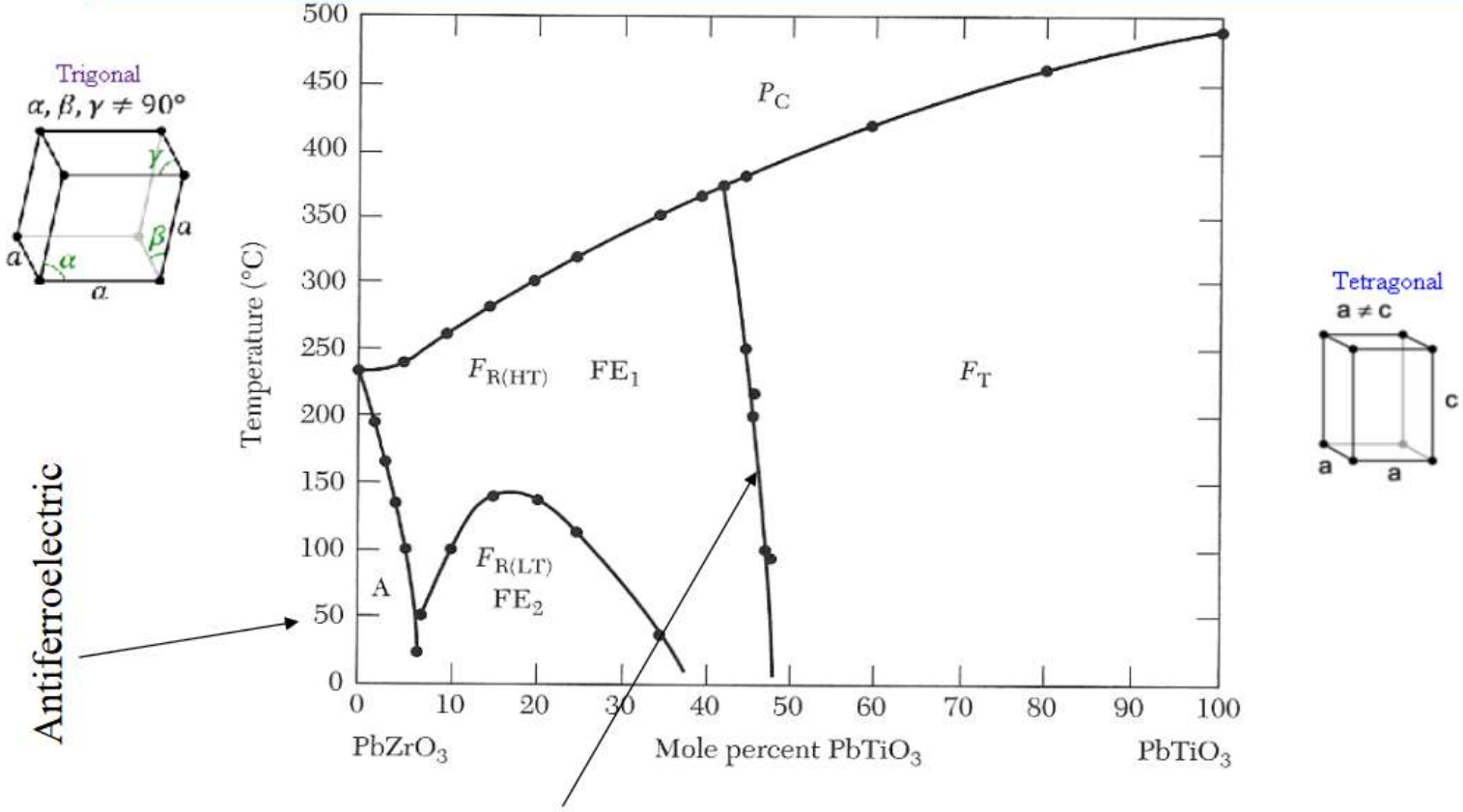


Can be used to make ultracapacitors





PZT ($Pb[Zr_xTi_{1-x}]O_3$ $0<x<1$)



Large piezoelectric response near the rhombohedral-tetragonal transition.
Electric field induces a structural phase transition.

Nitinol

Ni Ti alloy

Shape memory: If it is bent below a certain transition temperature and then heated above that temperature, it returns to its original shape.

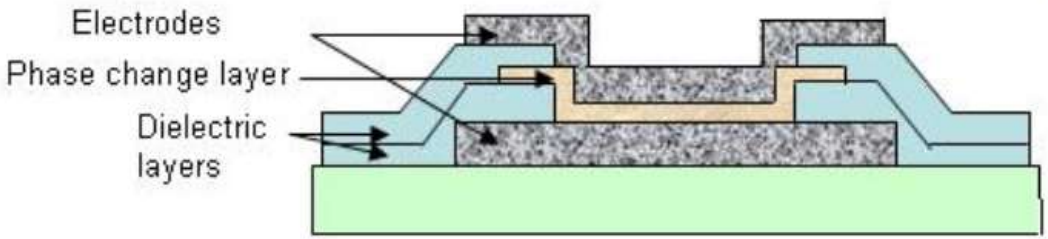
Superelasticity: Just above the transition temperature, the material exhibits elasticity 10-30 times that of an ordinary metal.

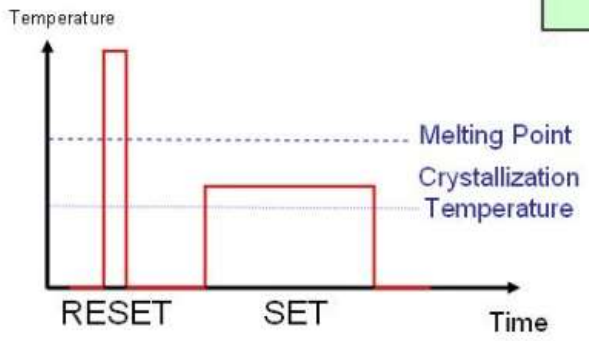
Martisite - Austinite

Phase change memory

Phase-change memory (PRAM) uses chalcogenide materials. These can be switched between a low resistance crystalline state and a high resistance amorphous state.

GeSbTe is melted by a laser in rewritable DVDs and by a current in PRAM.

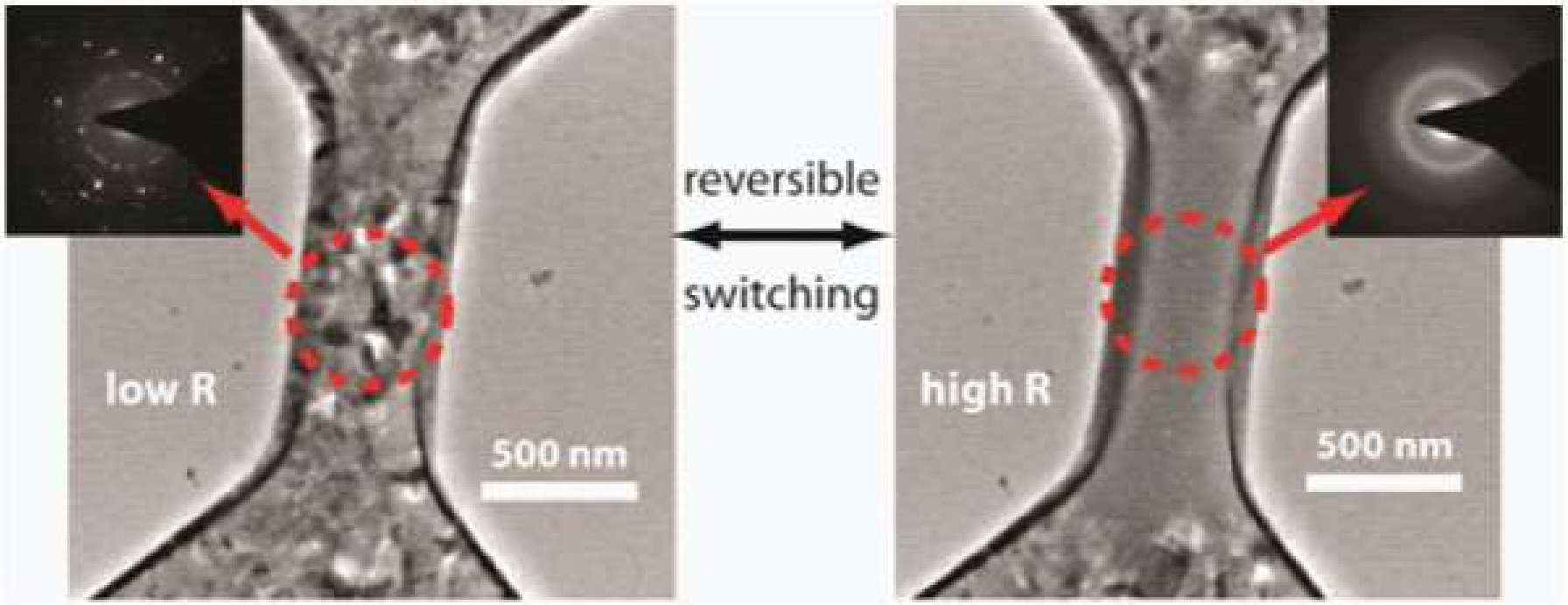




nonvolatile

Phase change material

Electron diffraction in a TEM of a GeSbTe alloy.



http://web.stanford.edu/group/cui_group/research.htm

doi:10.1016/j.calphad.2008.07.009
Cite or Link Using DOI

The surprising role of magnetism on the phase stability of Fe (Ferro)

1. Introduction

The phase stability of many elements shows the following pattern:

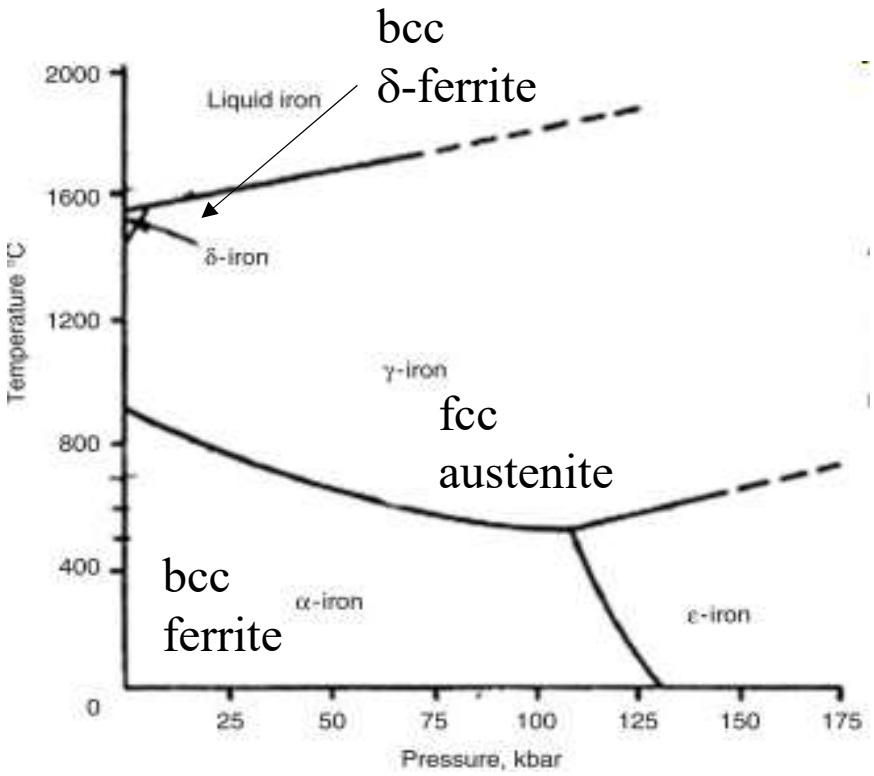
1. A low enthalpy is mainly responsible for the choice of structure at low temperatures.

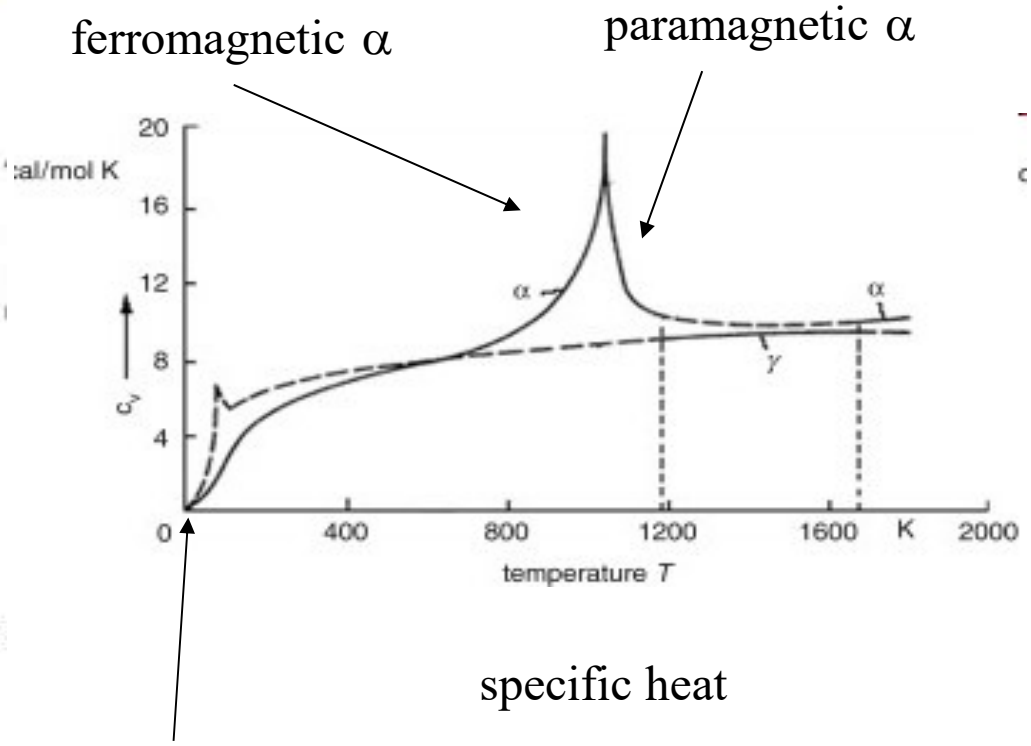
2. At higher temperatures, structures (phases) are stable which have higher entropies.

This often translates into the low temperature phase being a close packed one and the high temperature phase having a more open structure, that is, a less close packed structure. For example, the low temperature phase of Ti is close packed hexagonal (HCP) while the high temperature phase is BCC.

$$G = U + pV - TS$$

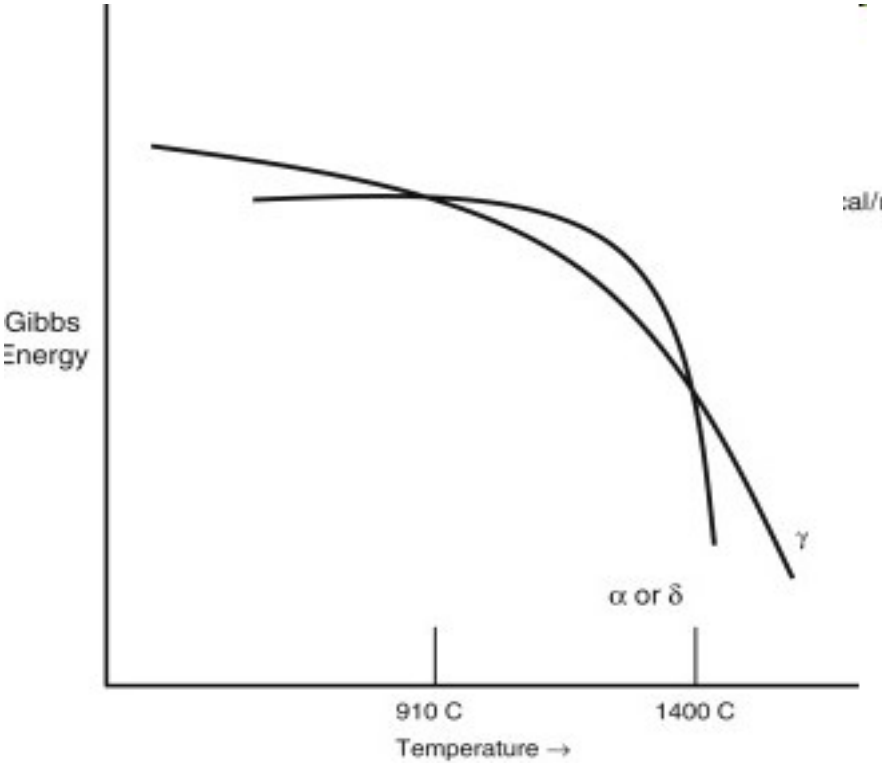
Structural phase transitions in iron

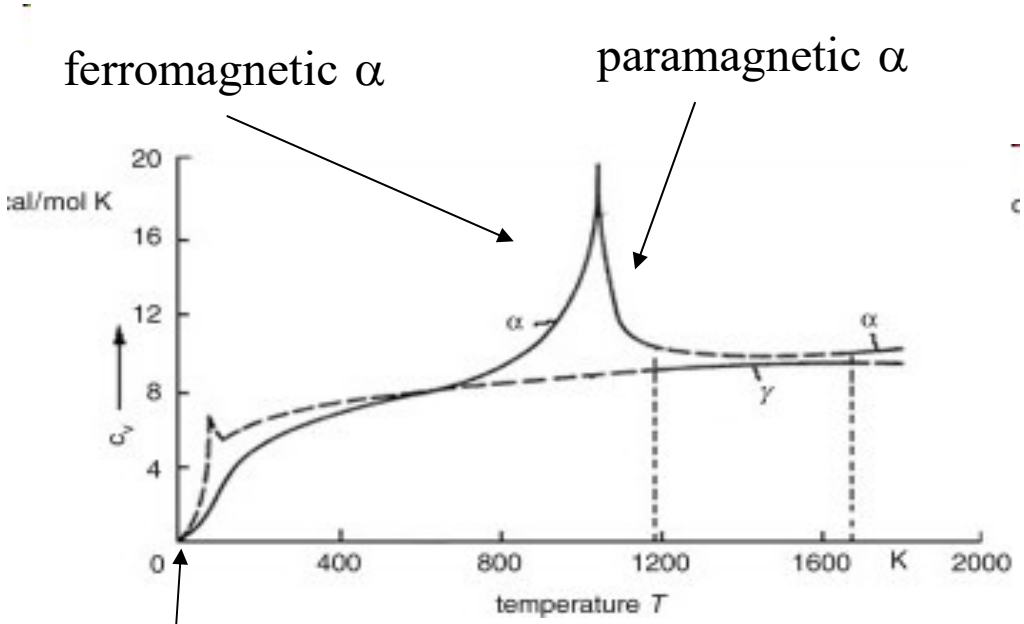




doi:10.1016/j.calphad.2008.07.009

Structural phase transitions in iron





doi:10.1016/j.calphad.2008.07.009

Iron alloy phases

Ferrite (α-iron, δ-iron)

Austenite (γ-iron)

Pearlite (88% ferrite, 12% cementite)

Martensite

Bainite

Ledeburite (austenite-cementite eutectic, 4.3% carbon)

Cementite (iron carbide, Fe_3C)

Beta ferrite (β-iron)

Hexaferrum (ε-iron)

Steel classes

Crucible steel

Carbon steel (≤2.1% carbon; low alloy)

Spring steel (low or no alloy)

Alloy steel (contains non-carbon elements)

Maraging steel (contains nickel)

Stainless steel (contains ≥10.5% chromium)

Weathering steel

Tool steel (alloy steel for tools)

Other iron-based materials

Cast iron (>2.1% carbon)

Ductile iron

Gray iron

Malleable iron

White iron

Wrought iron (contains slag)

v · d · e