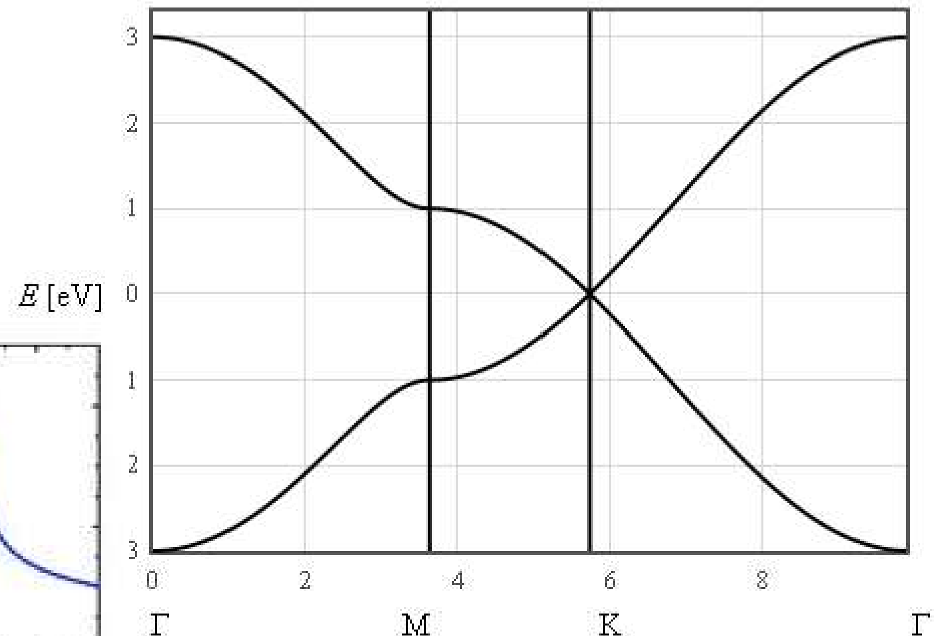
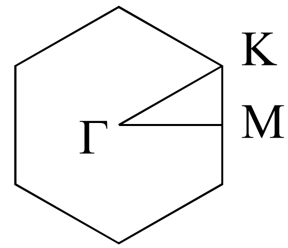
Some interesting materials

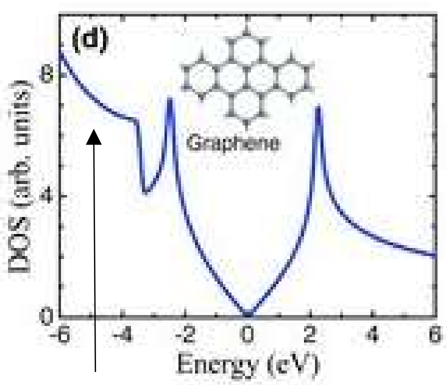
Tight binding dispersion relation for graphene

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

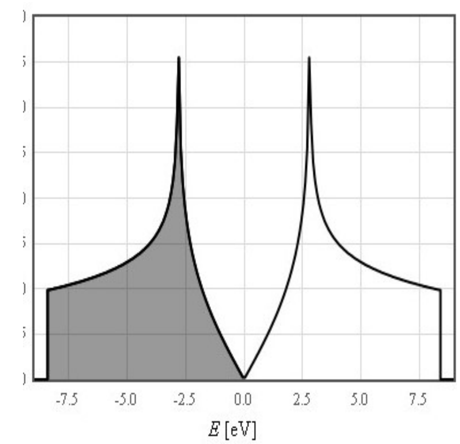




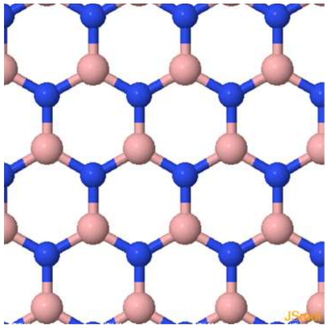
http://onlinelibrary.wiley.com/doi/10.1002/adfm.201101241/full



Another band is included here.

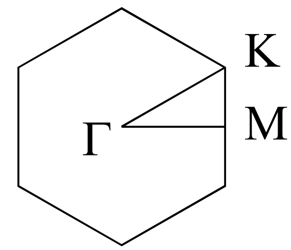


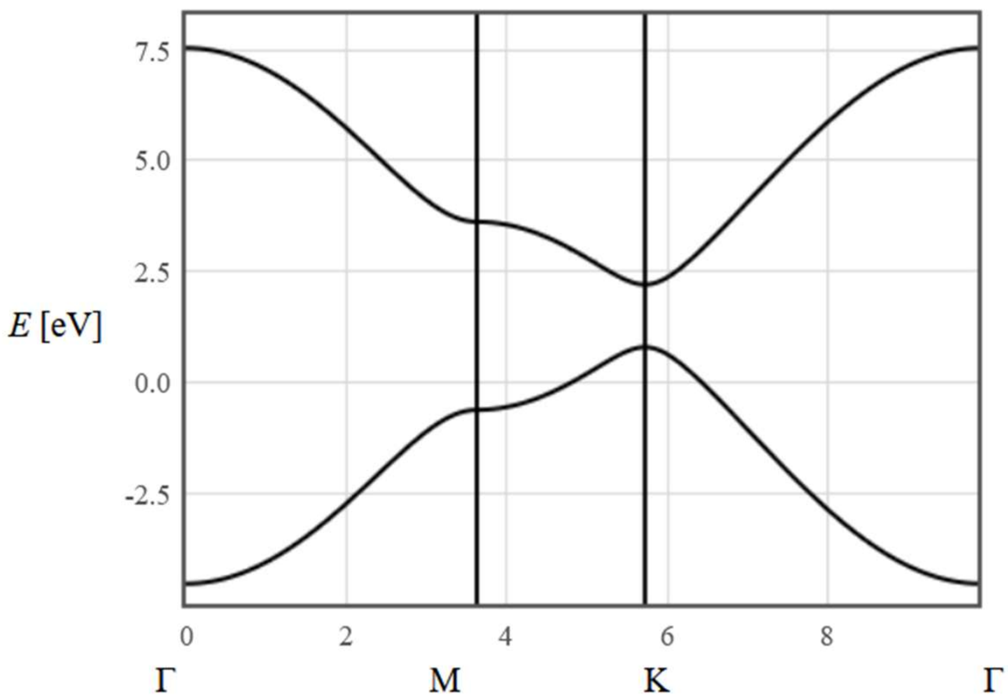
http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/dispgraphene.html

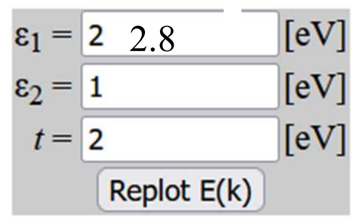


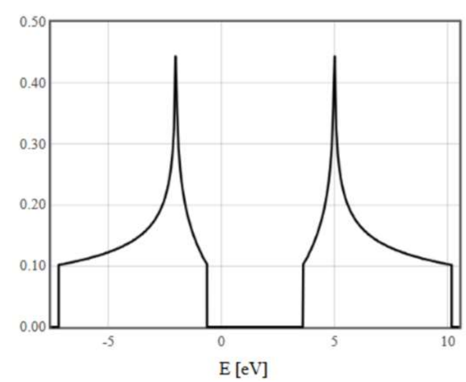
2-D boron nitride

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







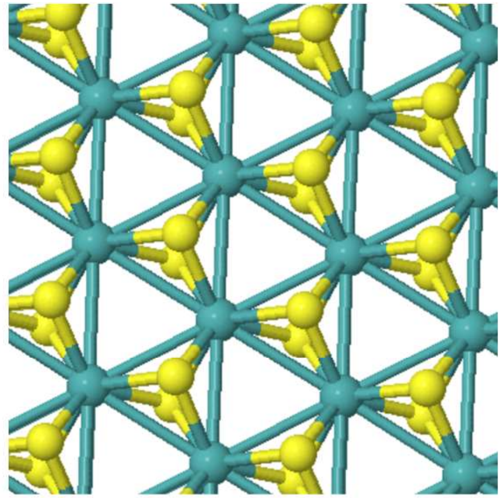


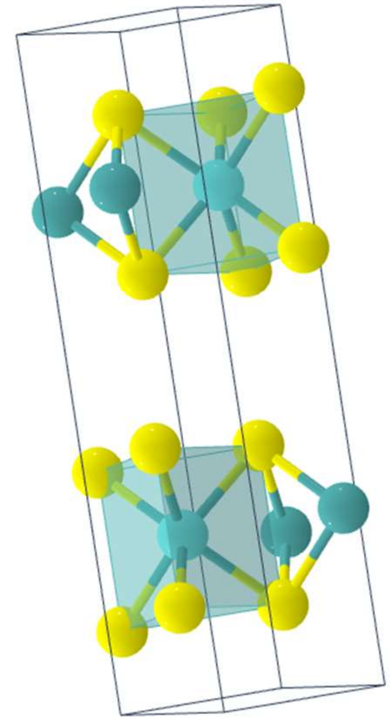
http://lampz.tugraz.at/~hadley/ss1/bands/tbtable/dispbn.html

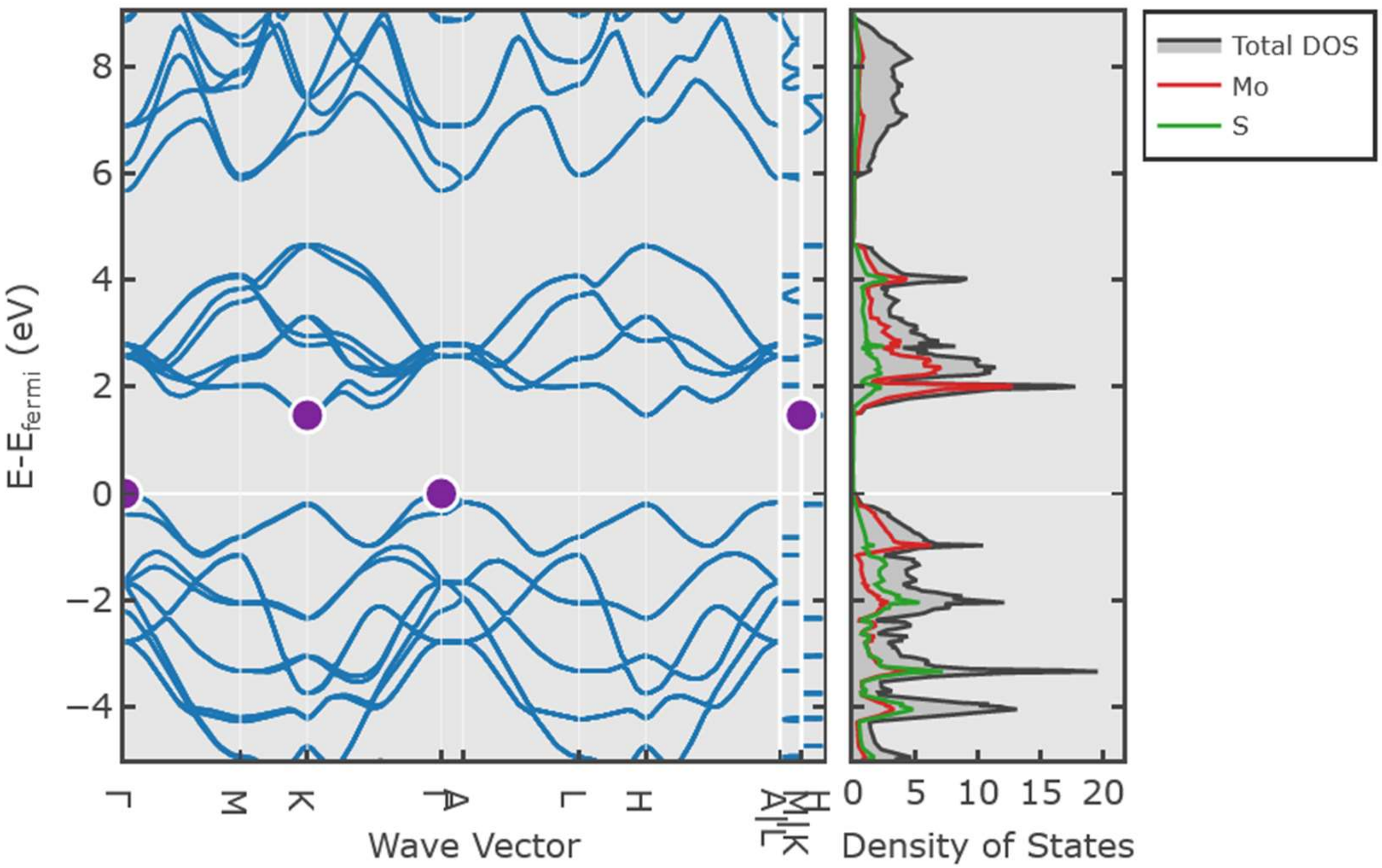
Materials Explorer

MoS_2

mp-2815

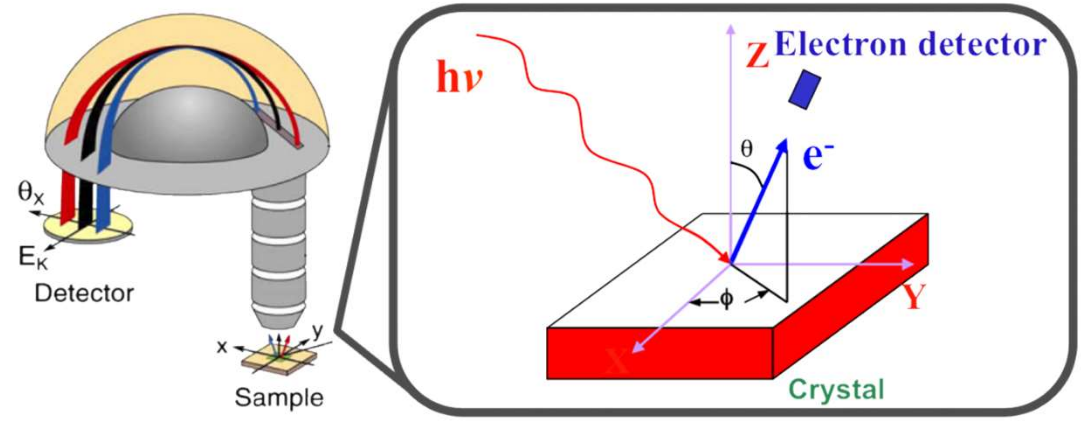




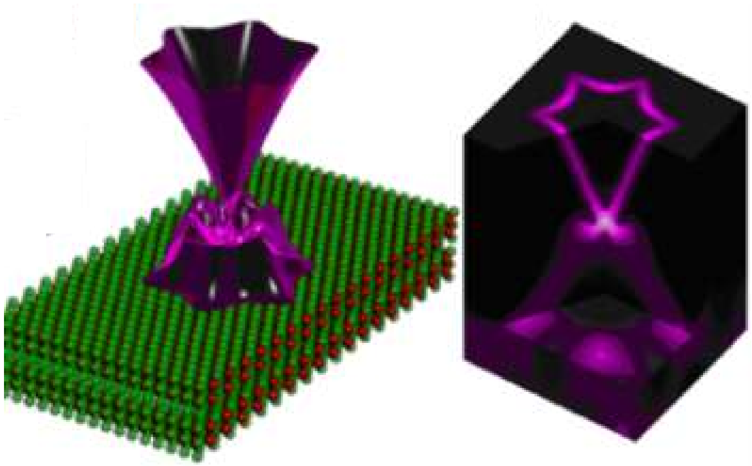


Angle resolved photoemission spectroscopy (ARPES)

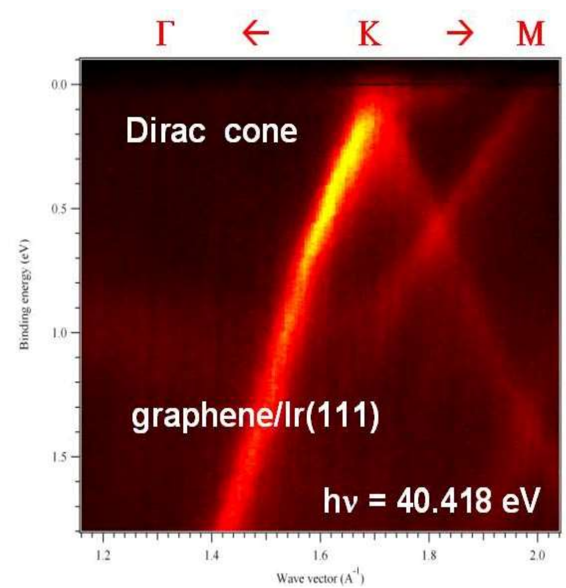
https://arpes.stanford.edu/research/tool-development/angle-resolved-photoemission-spectroscopy



Bi_2Te_3



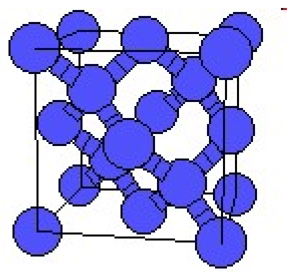
Topological insulator



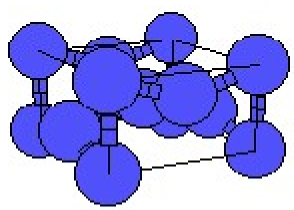
http://server2.phys.uniroma1.it/gr/lotus/Instrumentation1_M.htm

Measure the dispersion relation with angle resolved photoemission

Structural phase transitions

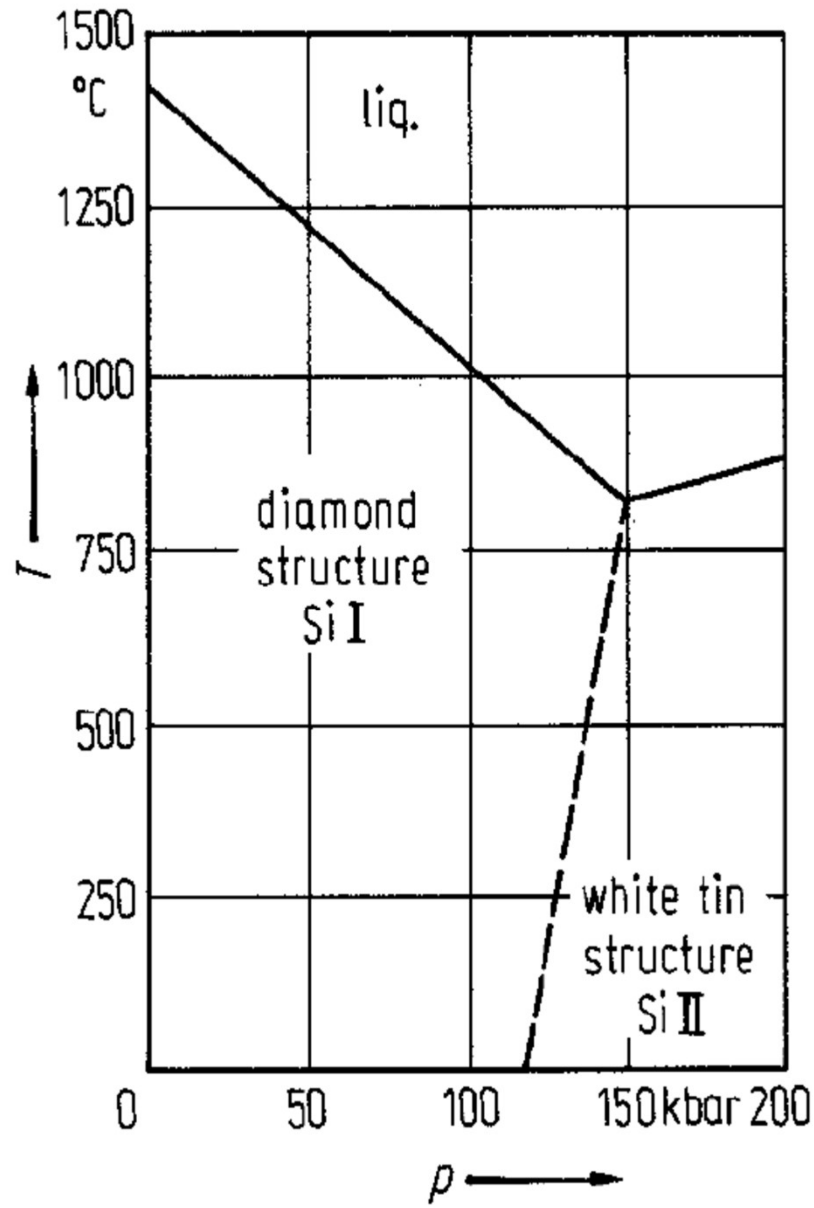


Si, diamond structure

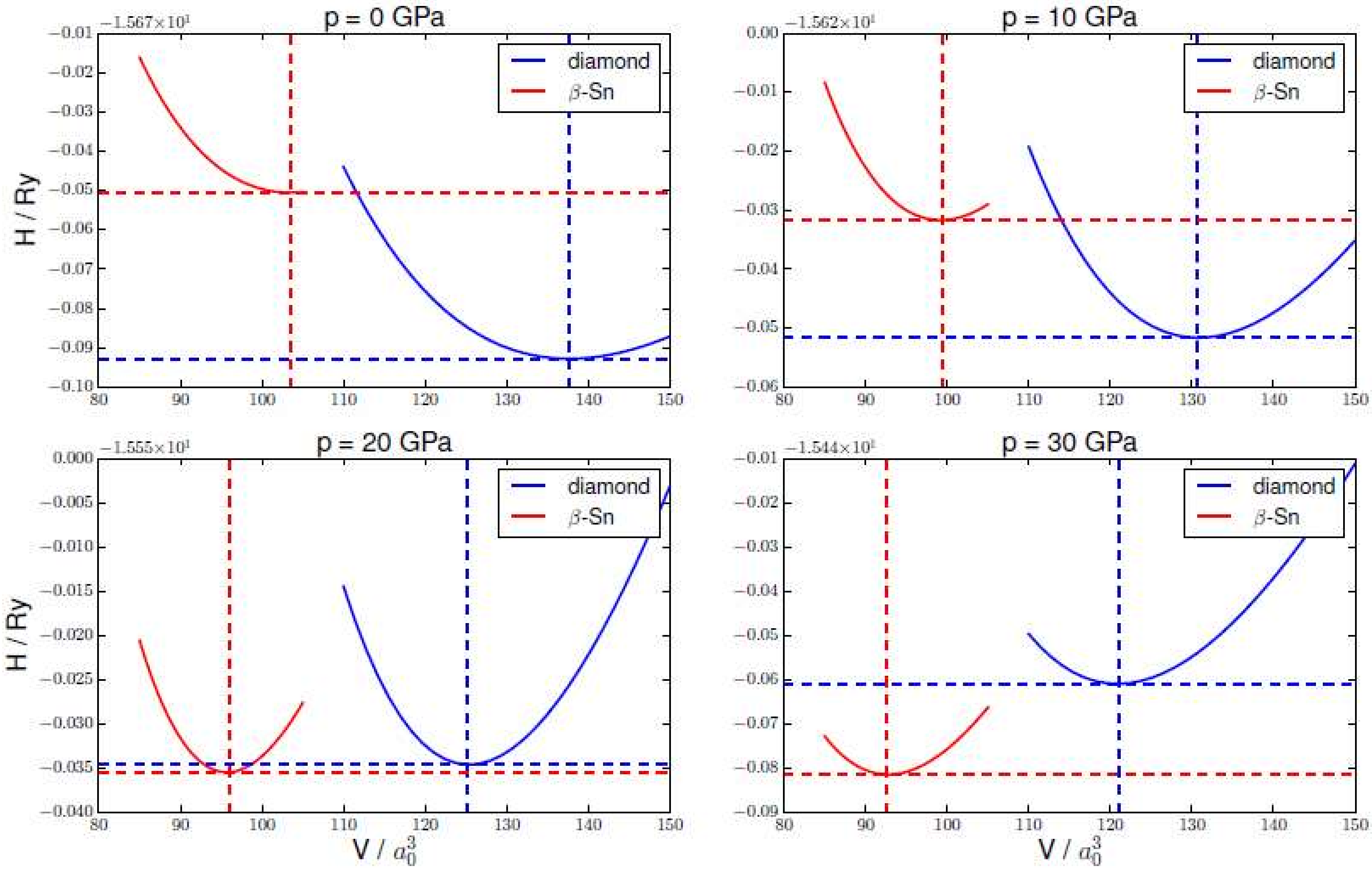


Si II, β-Sn, tetragonal

silicon makes a diamond to β-Sn transition under pressure



Structural phase transition in Si



Michael Scherbela 2015

Structural phase transition in Si

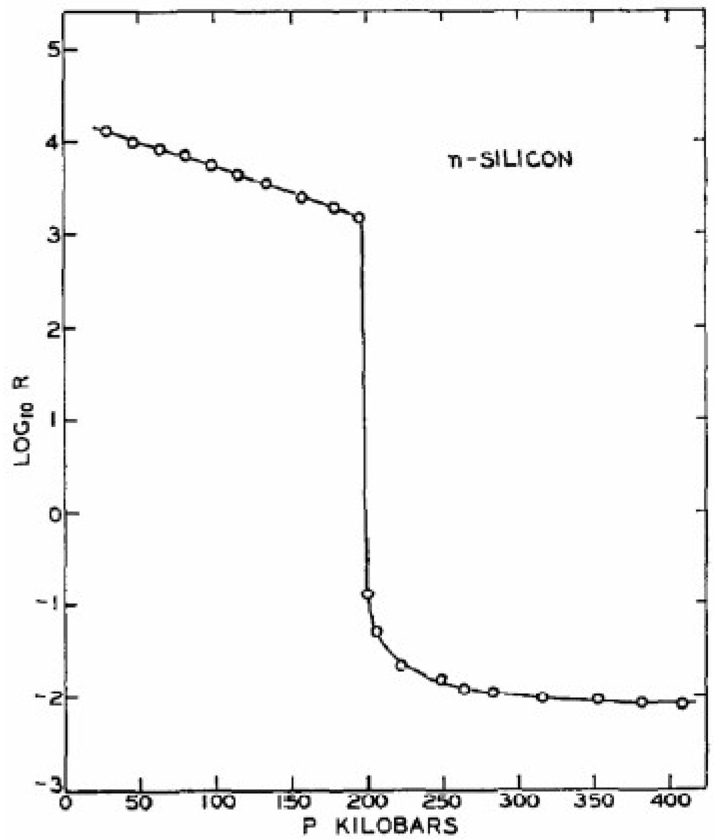
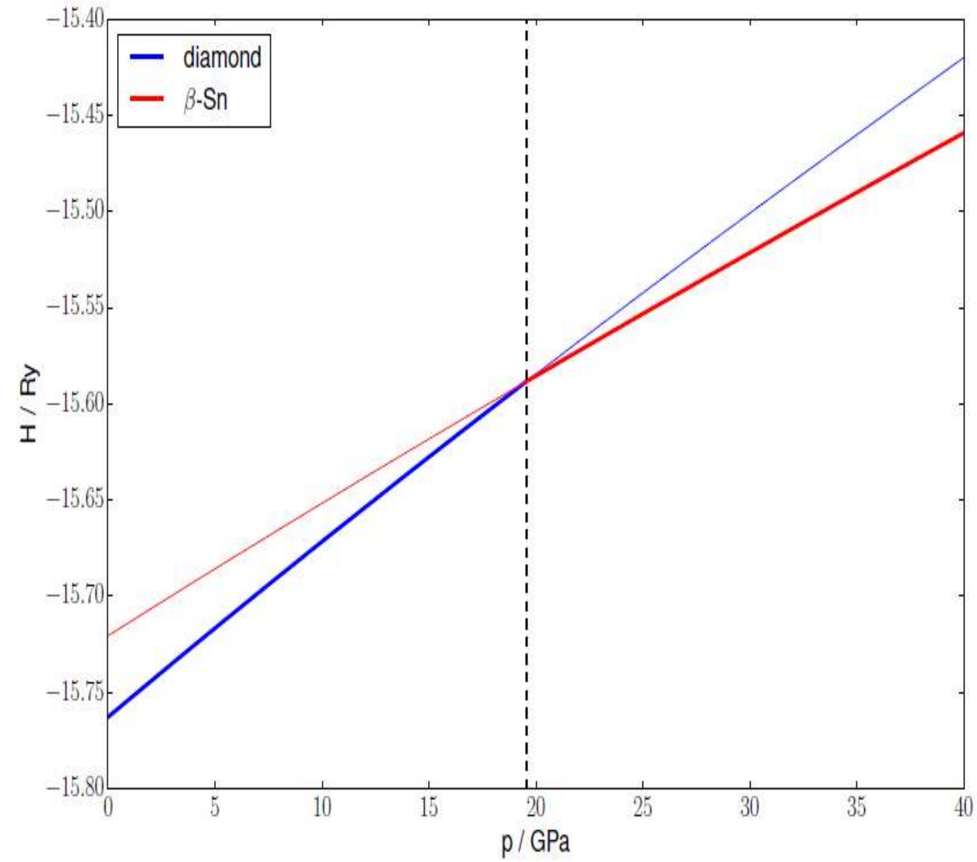


FIG. 1. Resistance vs. pressure—n-Silicon.



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.

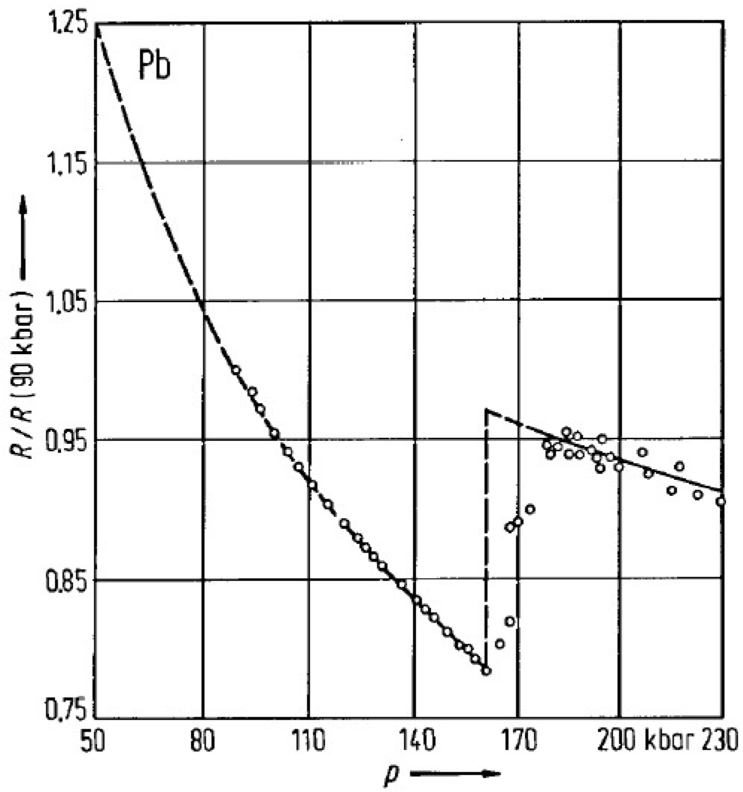
Strain

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.

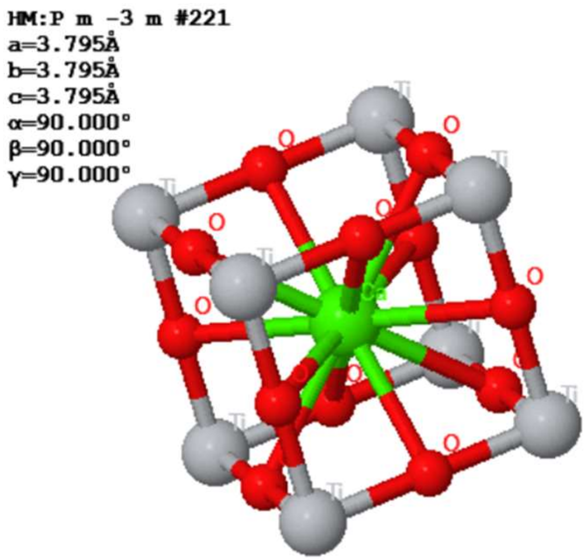
Enthalpy is calculated from the microscopic states of electrons and phonons.



Ferroelectricity

ABX$_3$

Perovskites

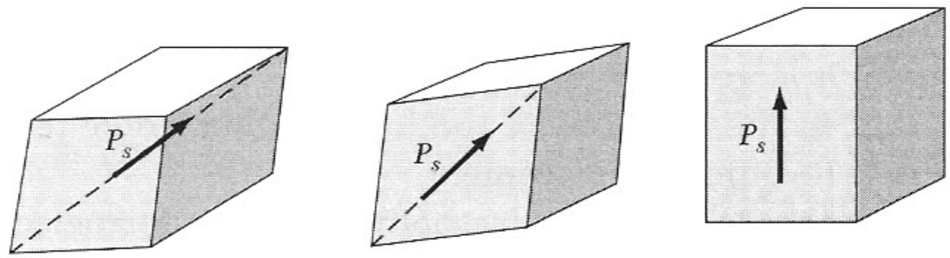


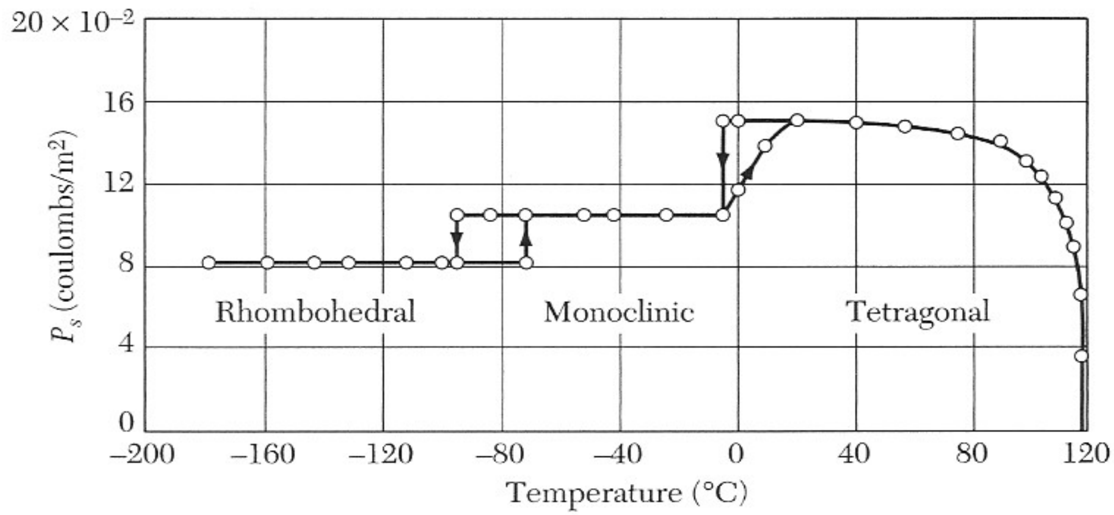
Spontaneous polarization
Analogous to ferromagnetism
Structural phase transition
T_c is transition temperature

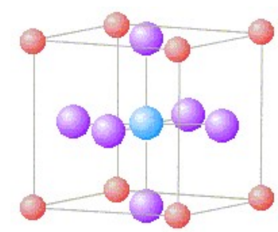
Electric field inside the material,
is not conducting

		T_c, in K	P_s, in $\mu C\ cm^{-2}$, 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]

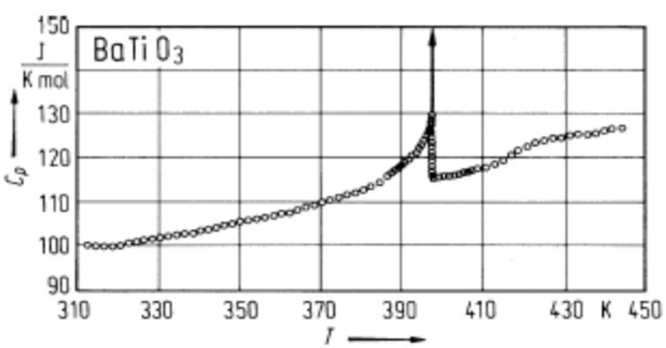
$BaTiO_3$







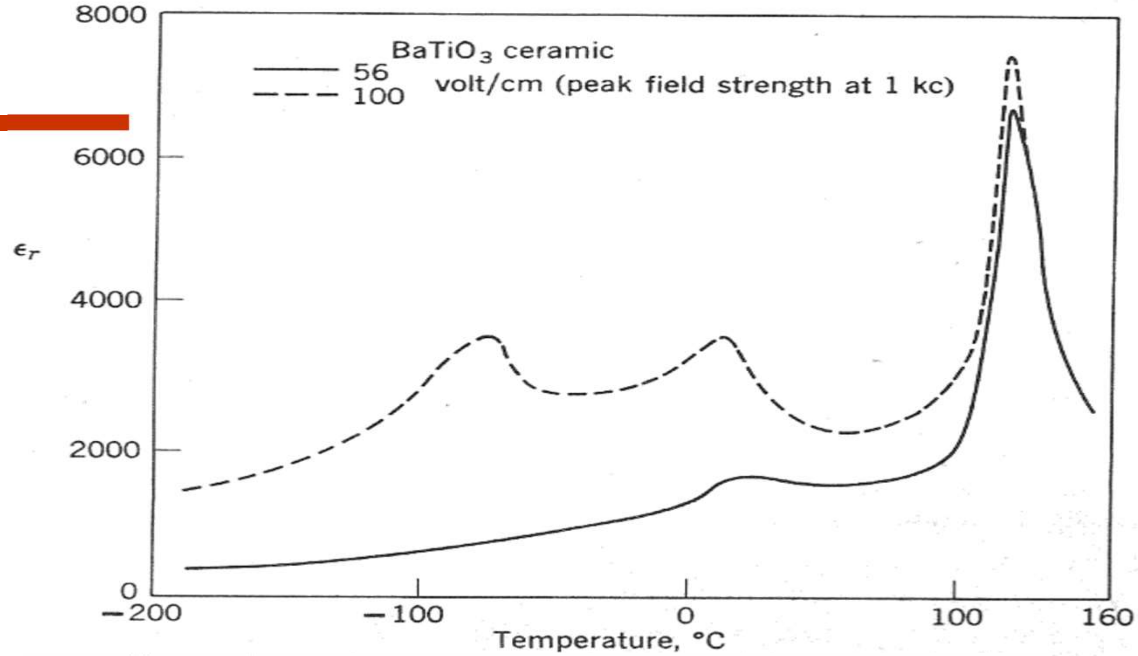
cubic (contains i => no spontaneous P)



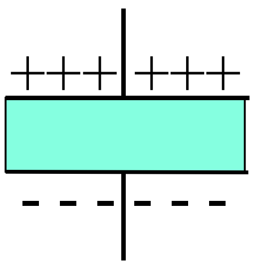
Can be used to make nonvolatile memory

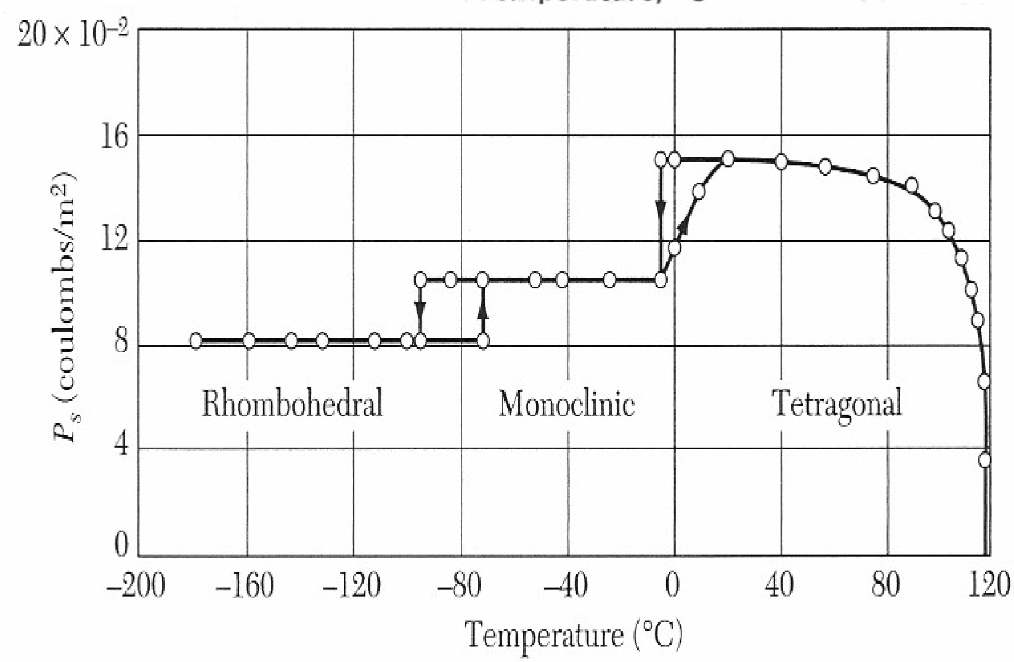
BaTiO$_3$

$$\varepsilon_r = \chi + 1$$



Can be used to make ultracapacitors

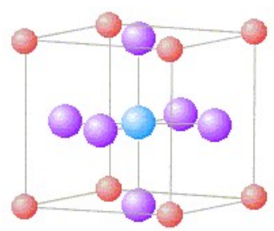


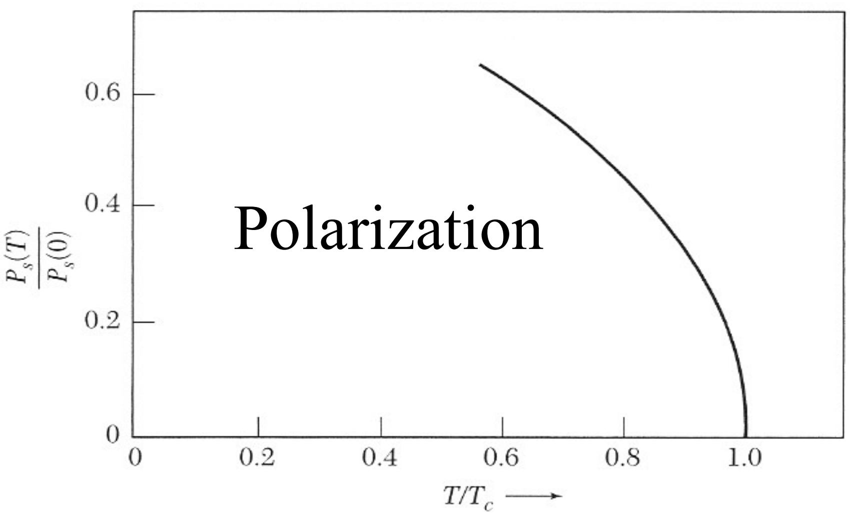


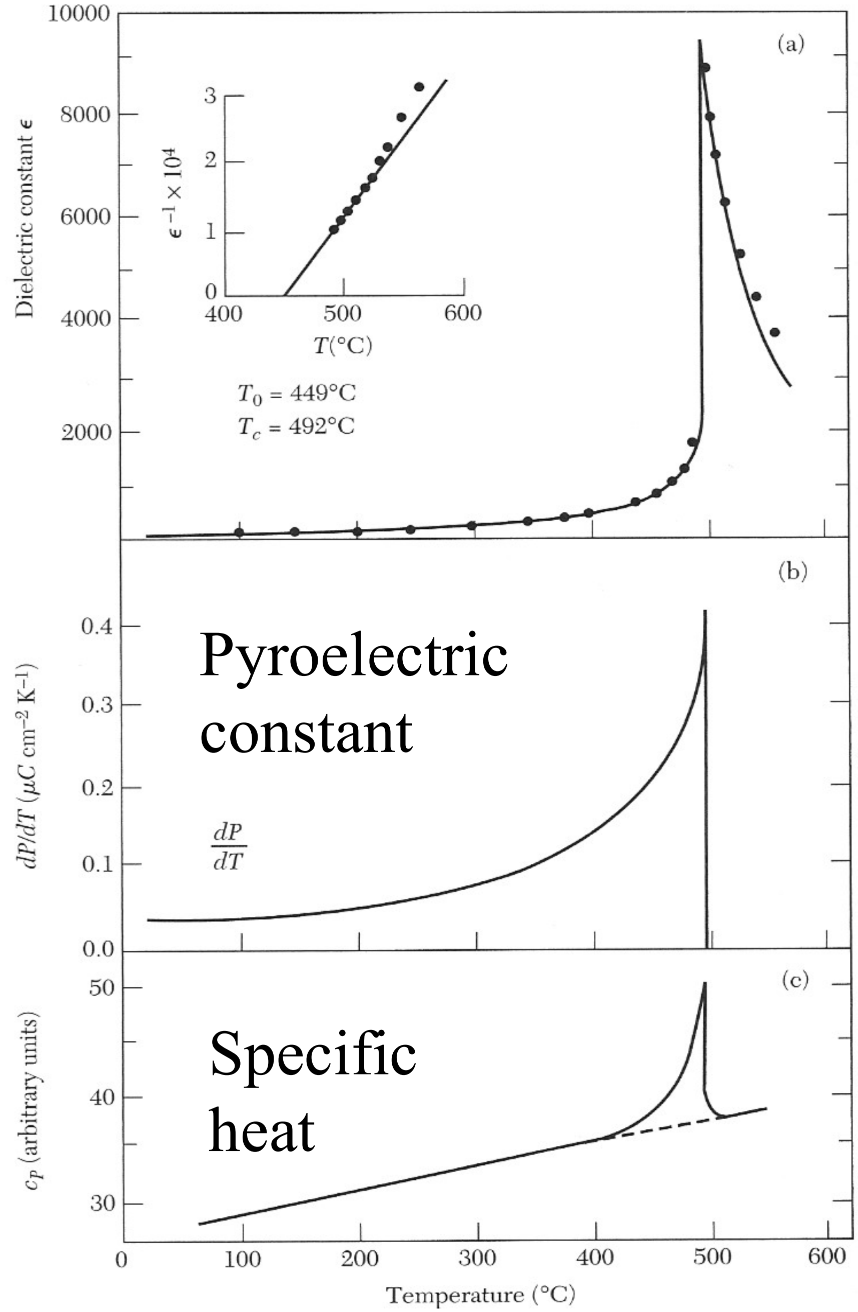
$PbTiO_3$

Dielectric constant

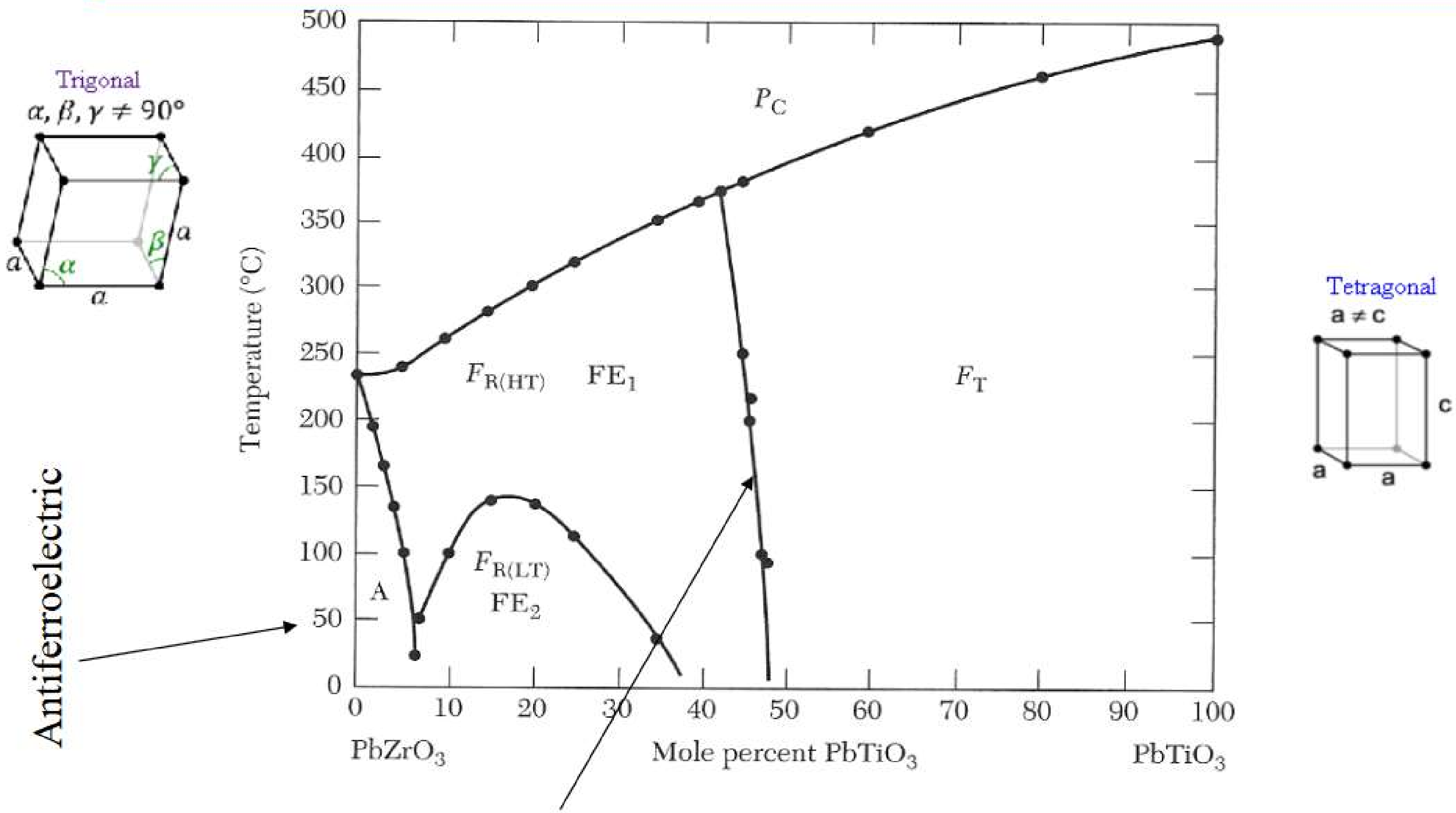
$$\varepsilon \propto \frac{1}{T - T_c}$$







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.

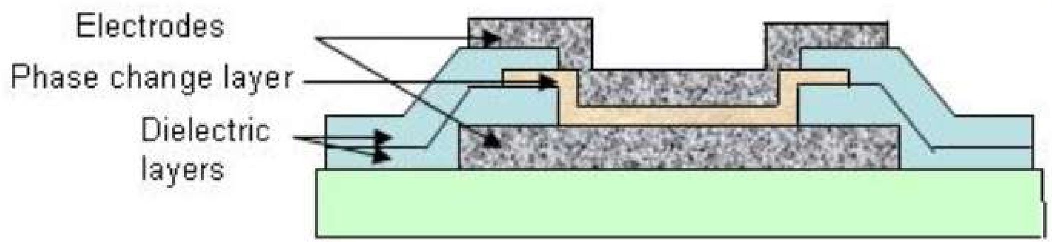
Superelasticity: Just above the transition temperature, the material exhibits elasticity 10-30 times that of an ordinary metal.

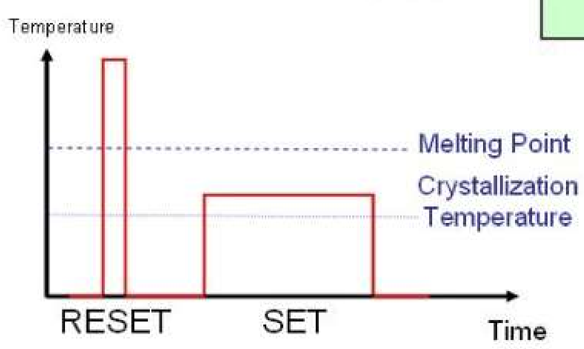
Martisite - Austinite

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.

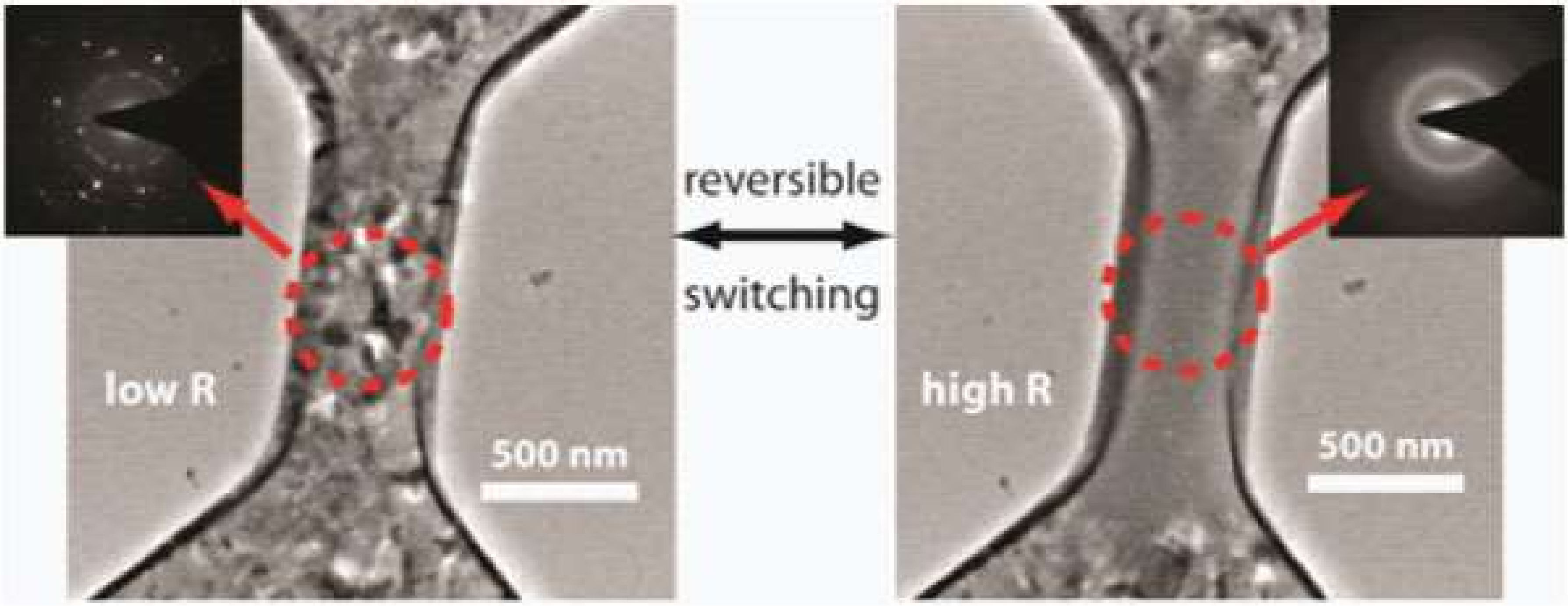




nonvolatile

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:

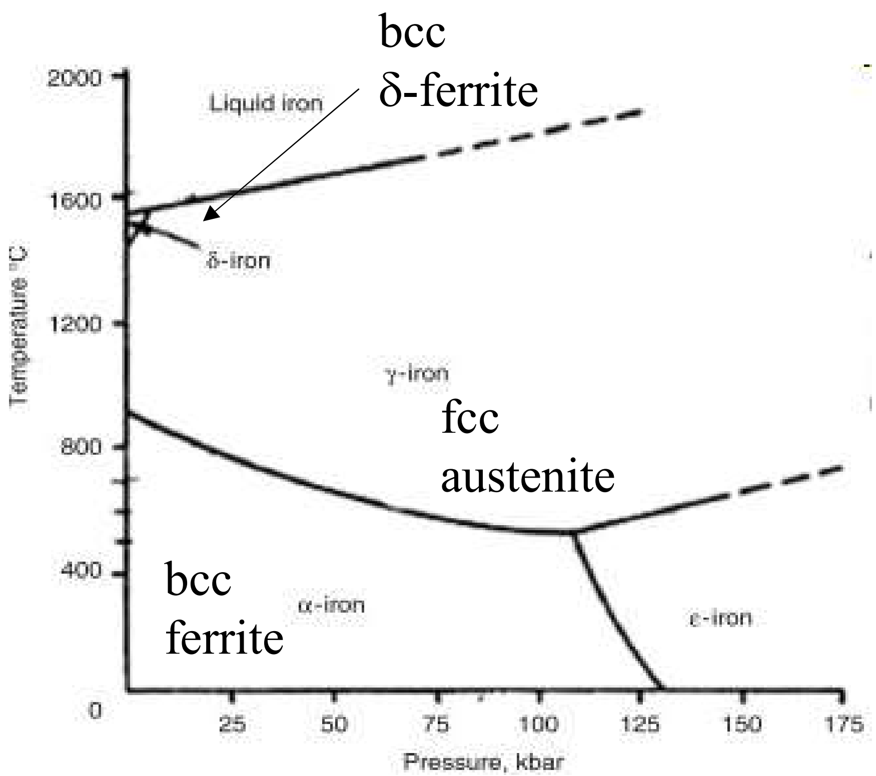
1. A low enthalpy is mainly responsible for the choice of structure at low temperatures.

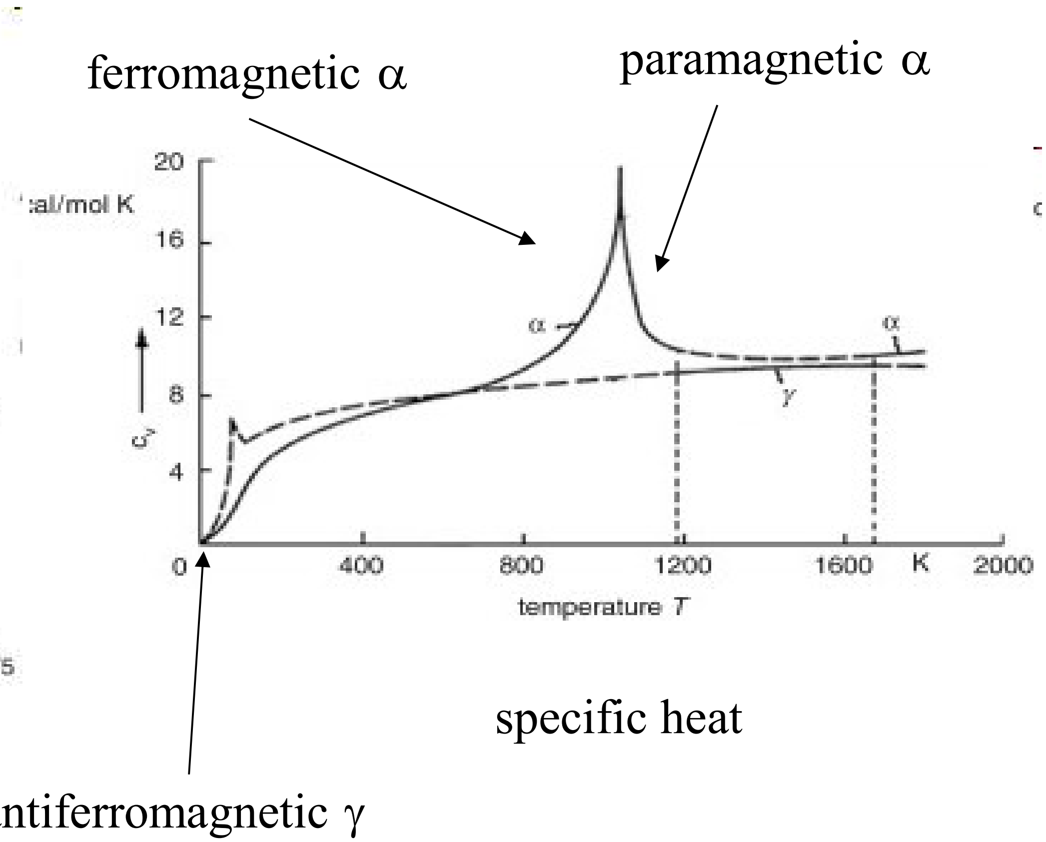
2. At higher temperatures, structures (phases) are stable which have higher entropies.

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

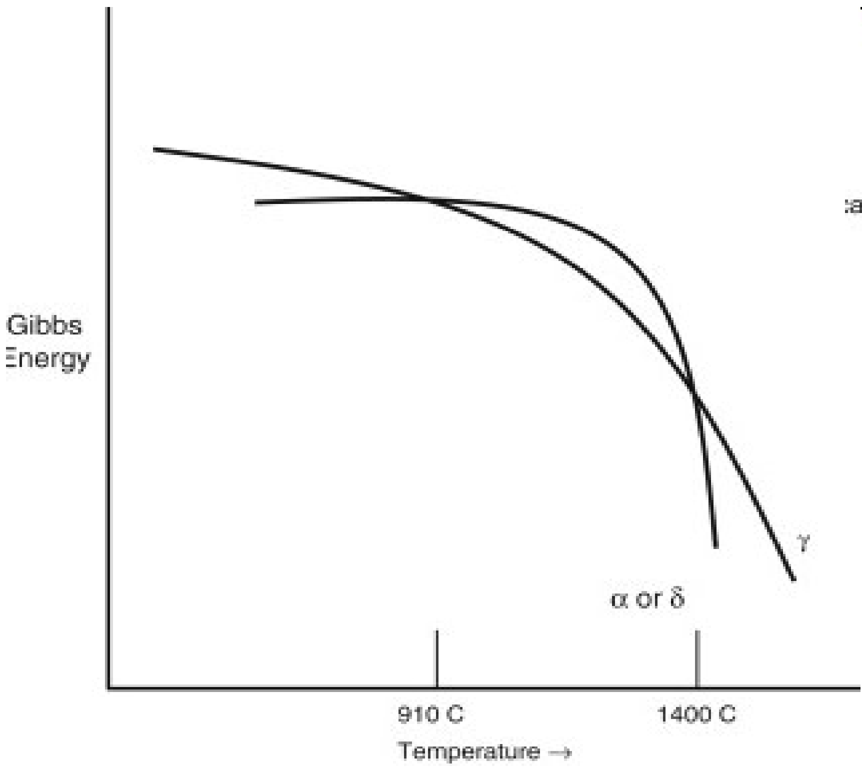




specific heat

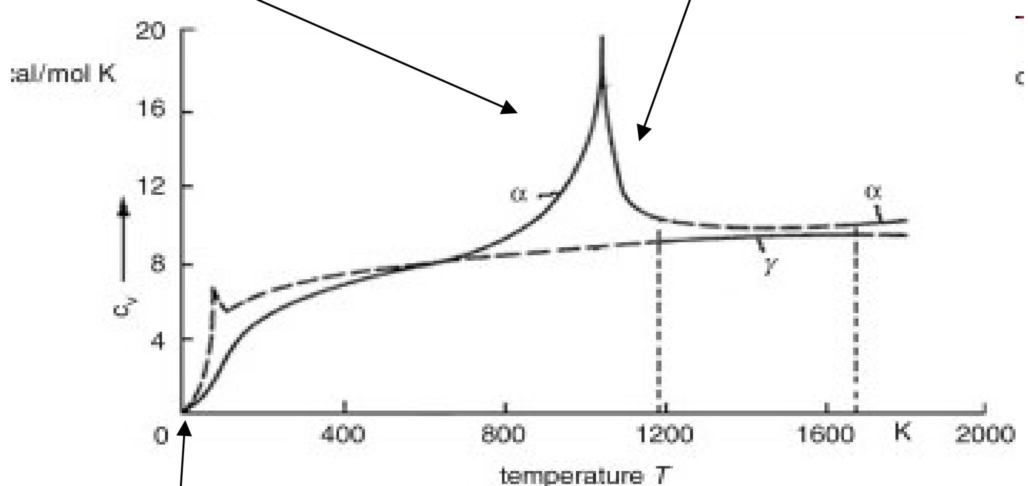
doi:10.1016/j.calphad.2008.07.009

Structural phase transitions in iron



ferromagnetic α

paramagnetic α



specific heat

antiferromagnetic γ

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)

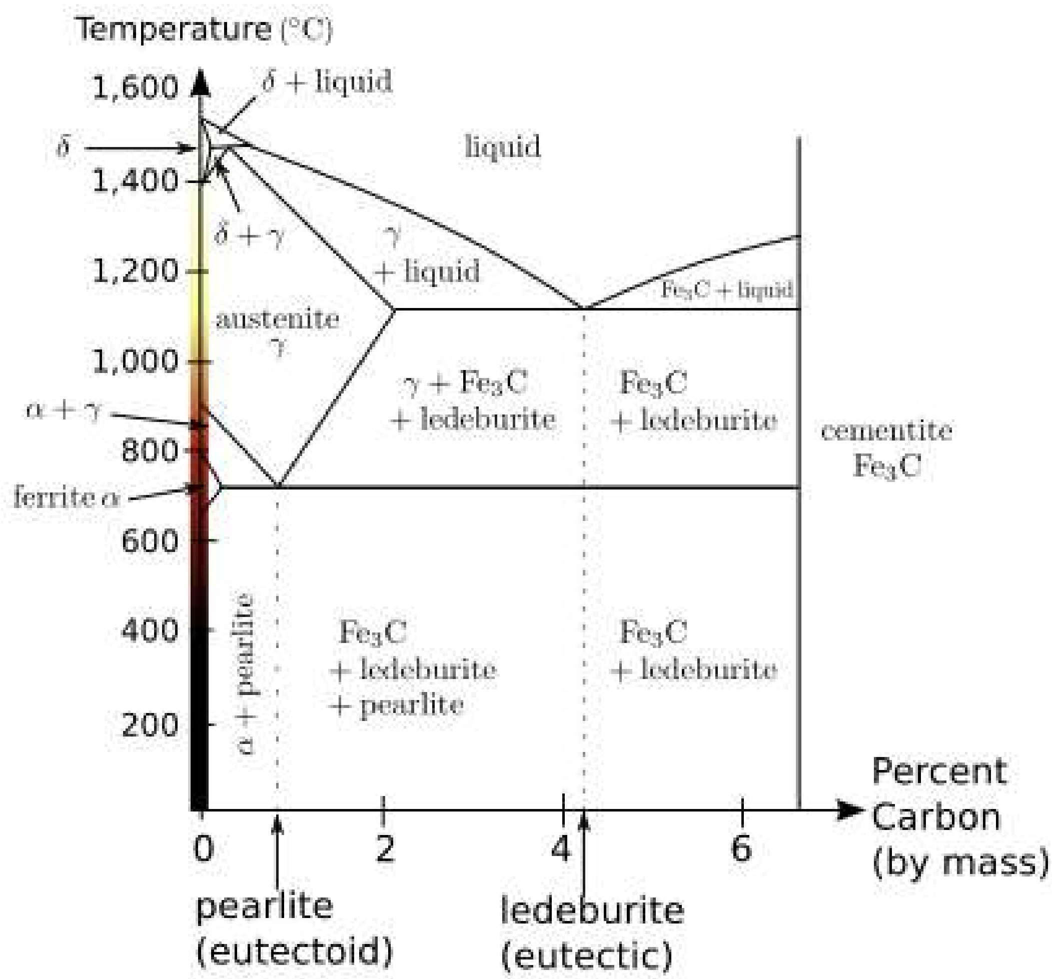
Steel classes

- 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)

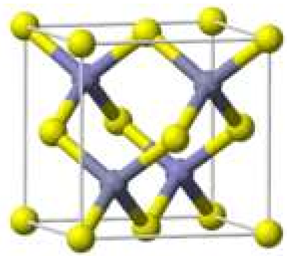
Other iron-based materials

- Cast iron (>2.1% carbon)
- Ductile iron
- Gray iron
- Malleable iron
- White iron
- Wrought iron (contains slag)

v · d · e

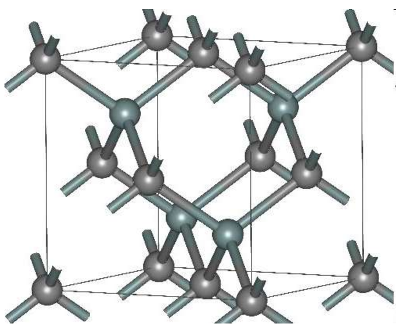


Structural phase transitions

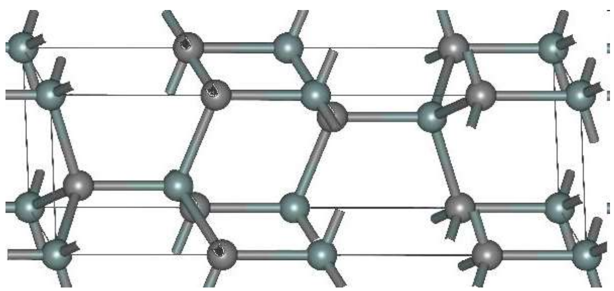


GaAs, Zincblende

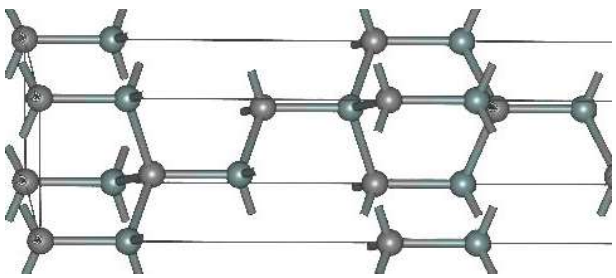
GaAs, Wurtzite



3C - SiC



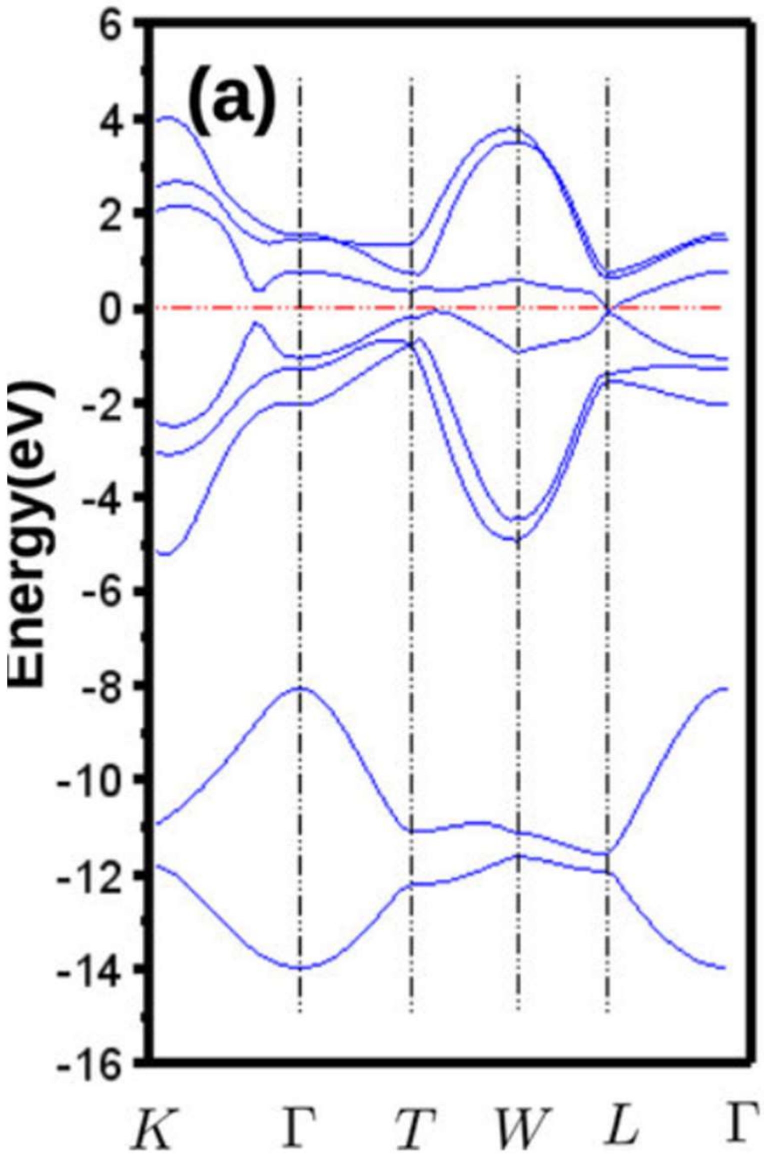
4H - SiC

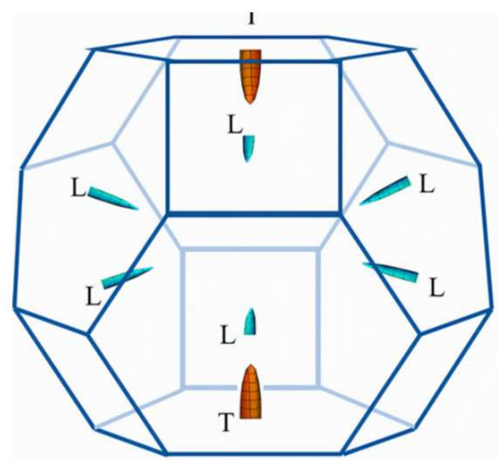


6H - SiC

SiC has about 100 polytypes

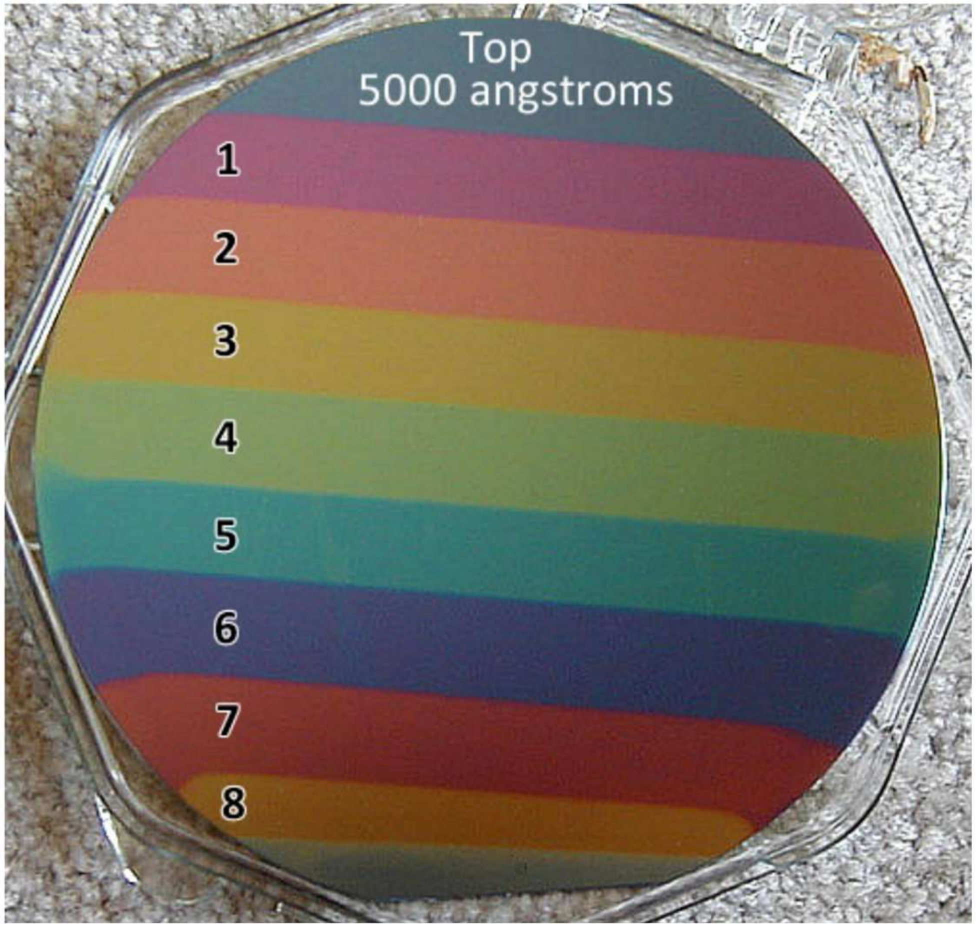
Bismuth



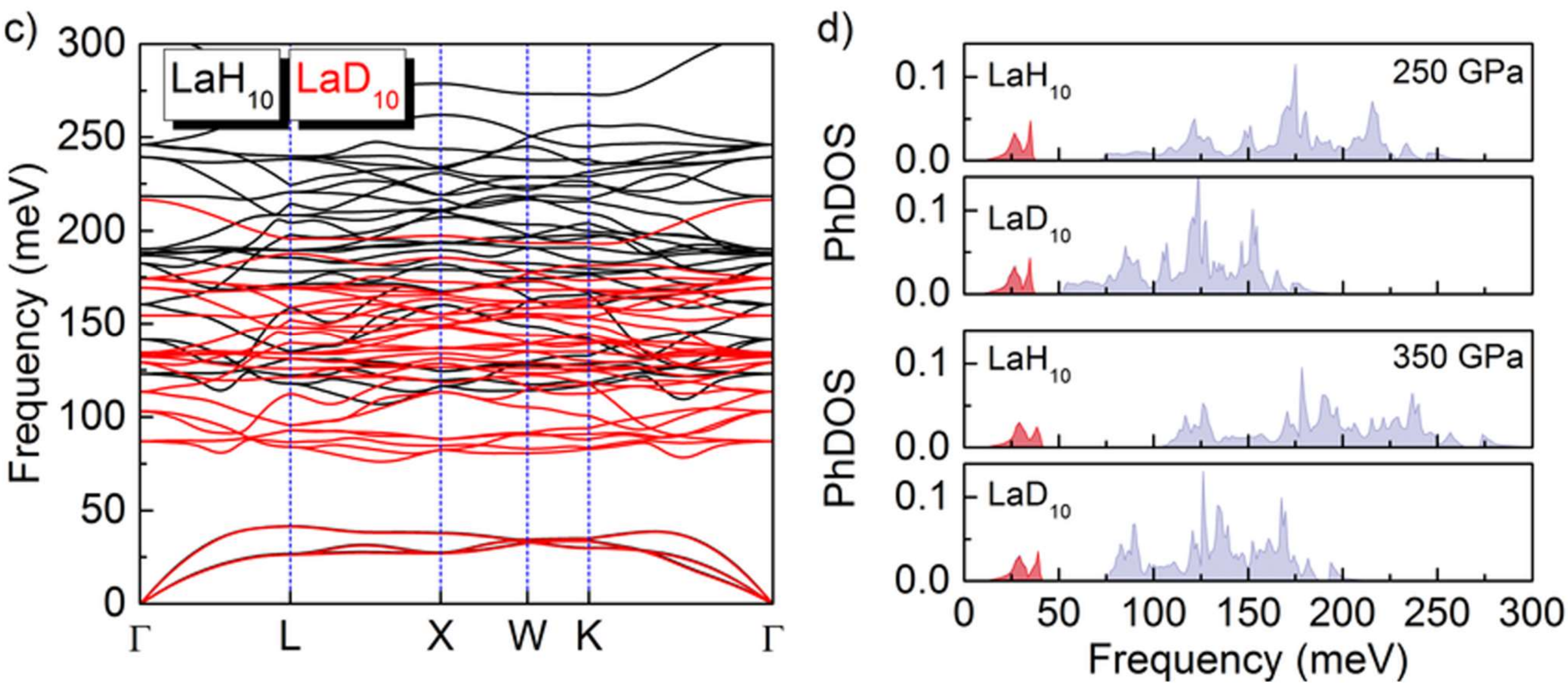


Kumar, Anil & Loke, Rajendra & Pramanik, Arindam & Sensarma, Rajdeep & Ramakrishnan, Sitaram & Prakash, Om & Bag, Biplab & Thamizhavel, Arumugam & Ramakrishnan, Srinivasan. (2022). 10.48550/arXiv.2212.03543.

SiO_2



Superconductivity in Hydrides



Quantum cascade laser