

Crystal structures

Crystal Structure

Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

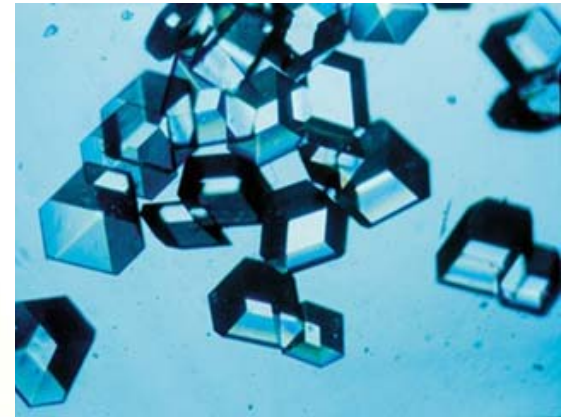
Many important materials (silicon, steel) are crystals



Gallium crystals

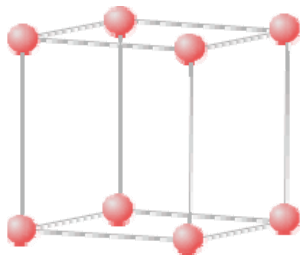
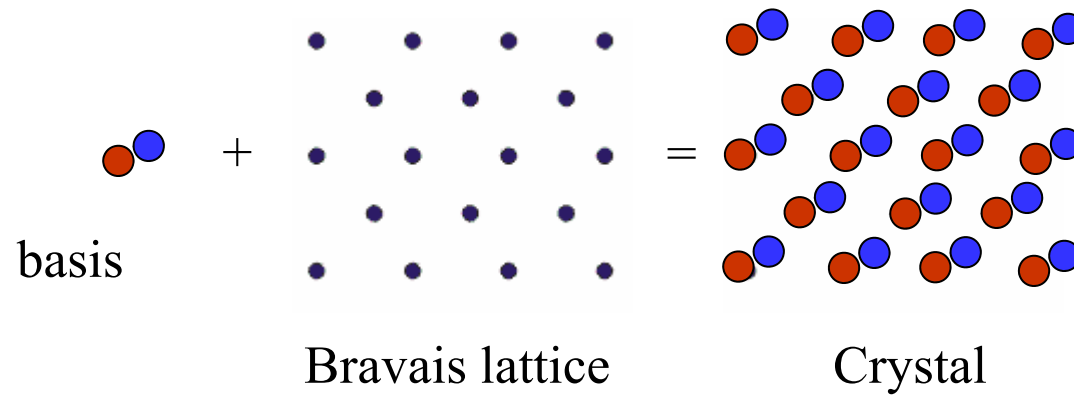


quartz

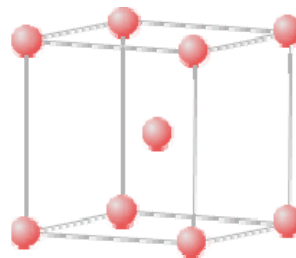


Insulin crystals

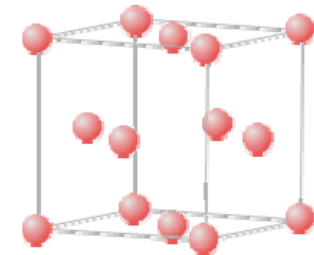
Crystal Structure



simple cubic

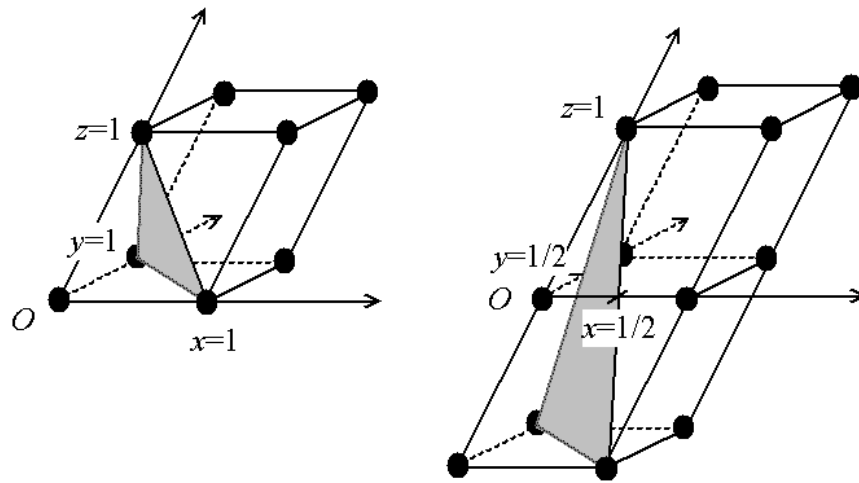
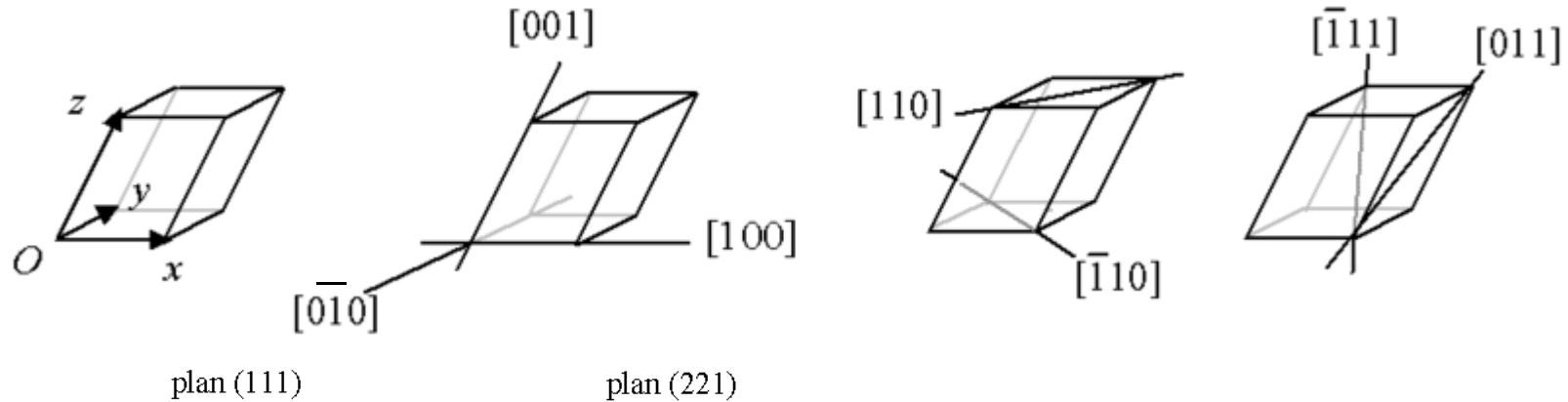


body centered
cubic, bcc



face centered
cubic, fcc

Crystal planes and directions: Miller indices



A plane with the intercepts $1/h$, $1/k$, $1/l$ is the (h,k,l) plane.

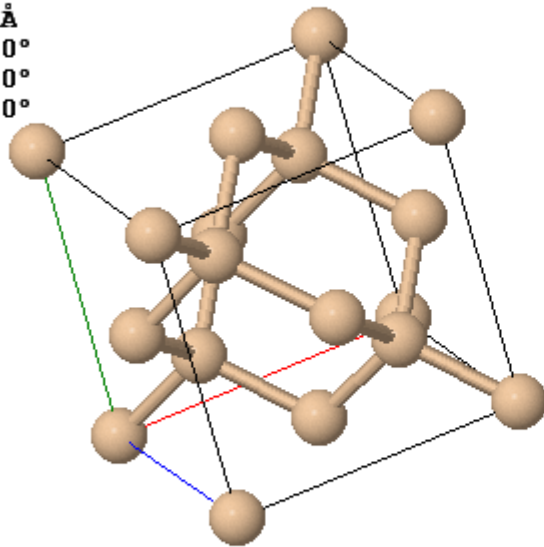
- [] specific direction
- < > family of equivalent directions
- () specific plane
- { } family of equivalent planes



MOSFETs are made on <100> wafers

silicon

HM: F d -3 m S
a=5.430Å
b=5.430Å
c=5.430Å
α=90.000°
β=90.000°
γ=90.000°



Conventional unit cell Primitive unit cell Asymmetric unit

2 x 2 x 2 3 x 3 x 3 5 x 5 x 5

Ball and Stick Spacefill

H: K: L:

show HKL plane hide HKL plane

draw atoms in HKL plane

Thickness of HKL planes:

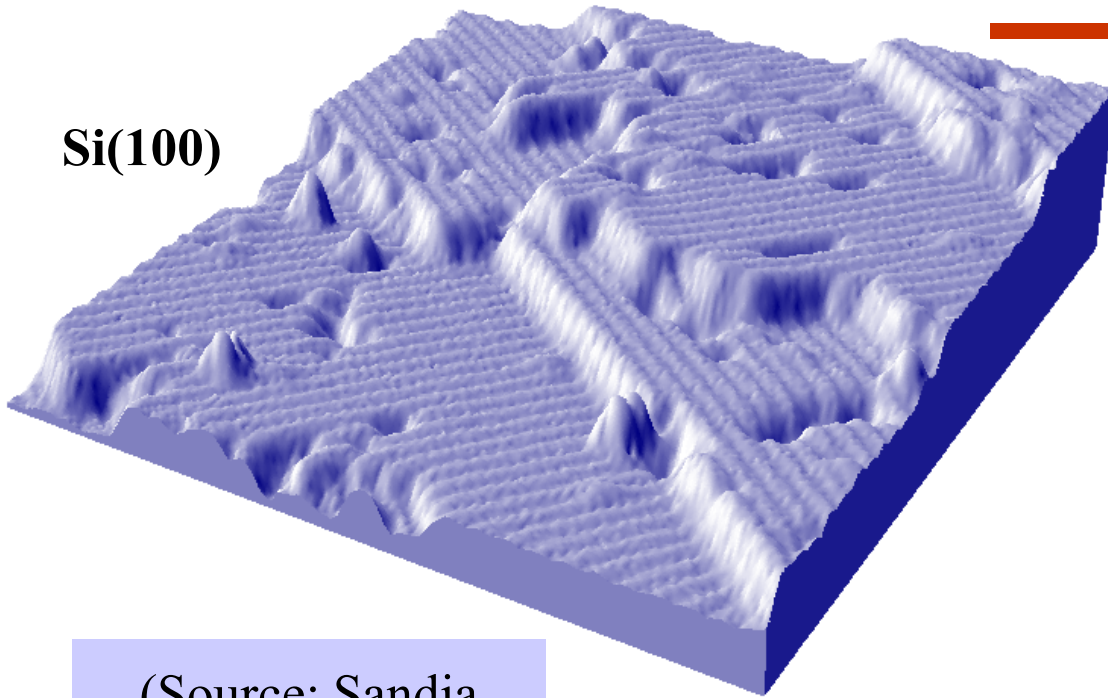
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

<http://lampx.tugraz.at/~hadley/memmm/materials/silicon/silicon.php>

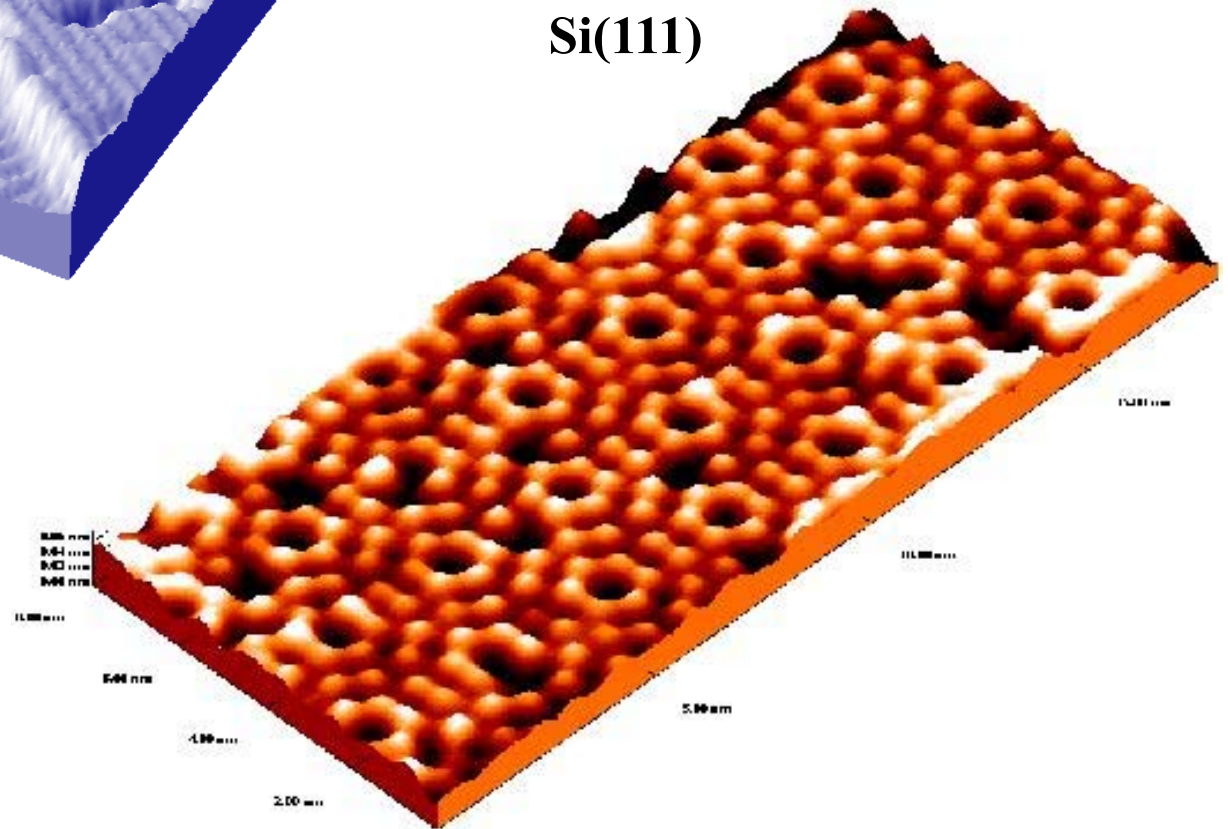
Silicon surfaces

Si(100)

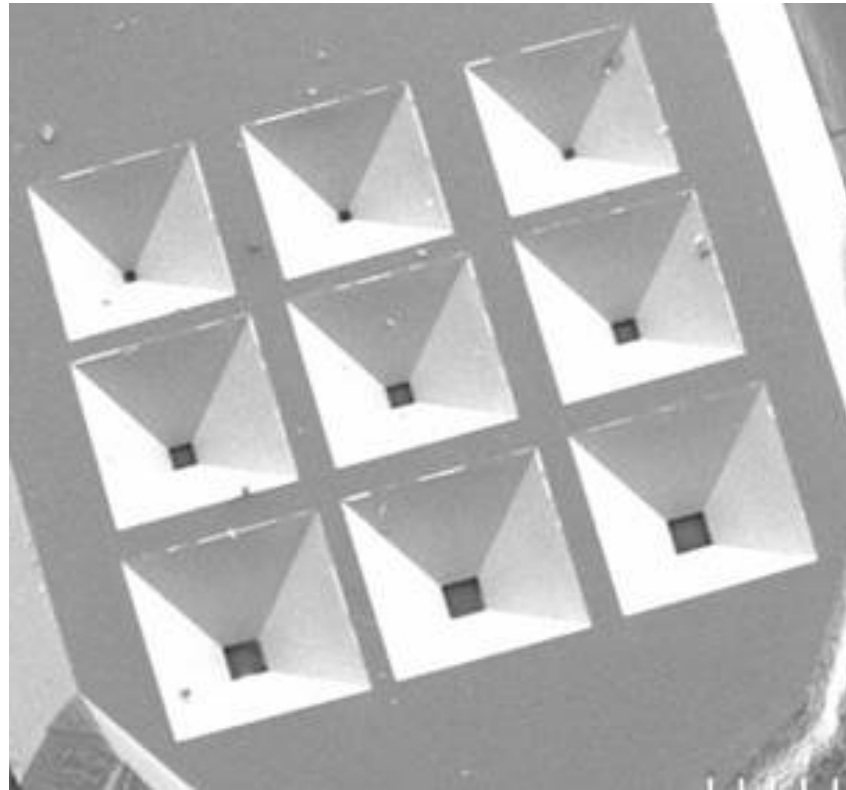


(Source: Sandia
Nat.Labs.)

Si(111)



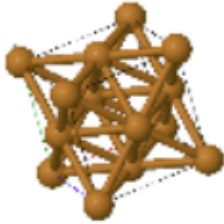
KOH etching of silicon



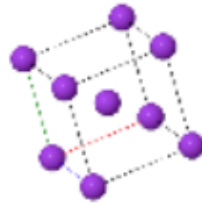
KOH etches Si $\{110\} > \{100\} > \{111\}$, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

http://www.ece.uncc.edu/research/clean_room/fabprocesses/KOH-EtchingAndDecon.pdf

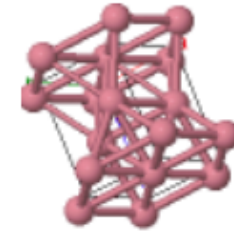
Crystal structures



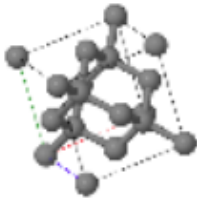
Face Centered
Cubic
Al, Cu, Ni, Ag, Pt, Au,
Pb



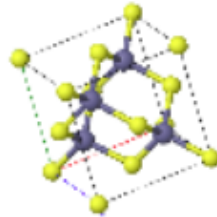
Body Centered
Cubic
W, Cr, Fe, Mo, Ta



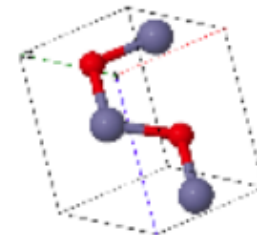
Hexagonal Close
Packed
Ti, Co, Zn, Zr



Diamond
C, Si, Ge, α -Sn



Zincblende
GaAs, InP, GaP, InAs,
AlAs

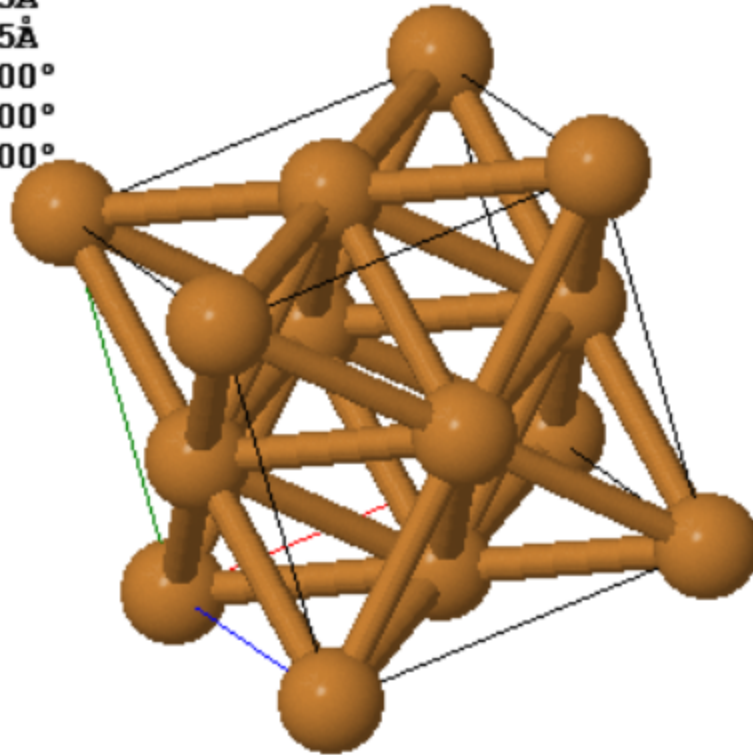


Wurtzite
ZnO, GaN, AlN, CdSe

face centered cubic (fcc)

Al, Cu,
Ni, Ag,
Pt, Au,
Pb

HM: $F m \bar{3} m$
 $a=3.615\text{\AA}$
 $b=3.615\text{\AA}$
 $c=3.615\text{\AA}$
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$

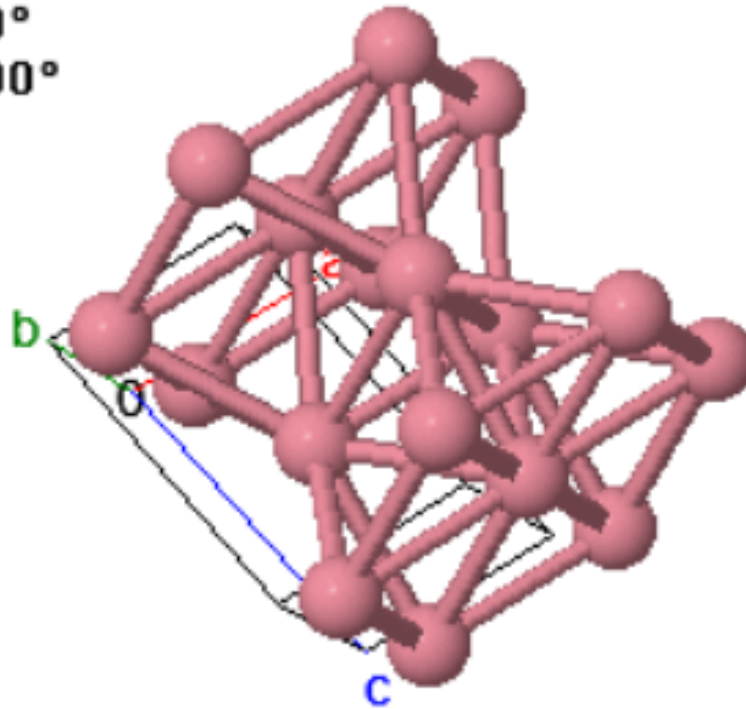


http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/fcc/fcc_jsmol.php

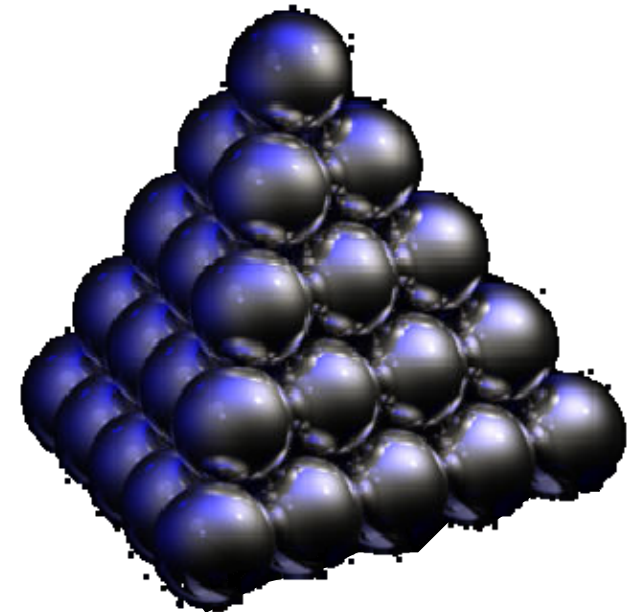
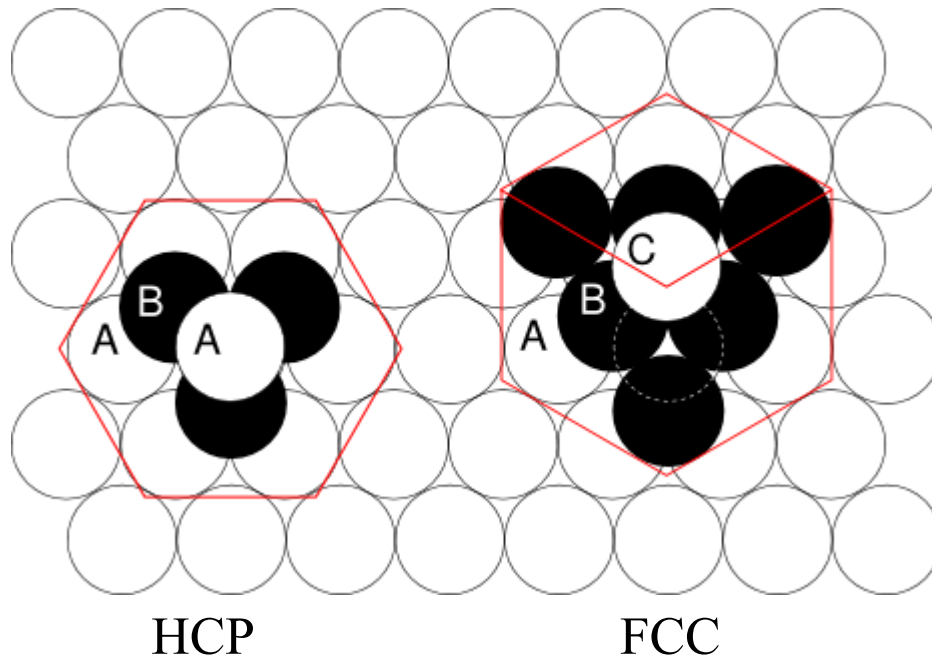
hexagonal close pack (hcp)

Ti, Co,
Zn, Zr,

HM: P 63/m m c
a=2.507Å
b=2.507Å
c=4.069Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=120.000^\circ$



Close packing



FCC = Face Centered Cubic ABCABC...

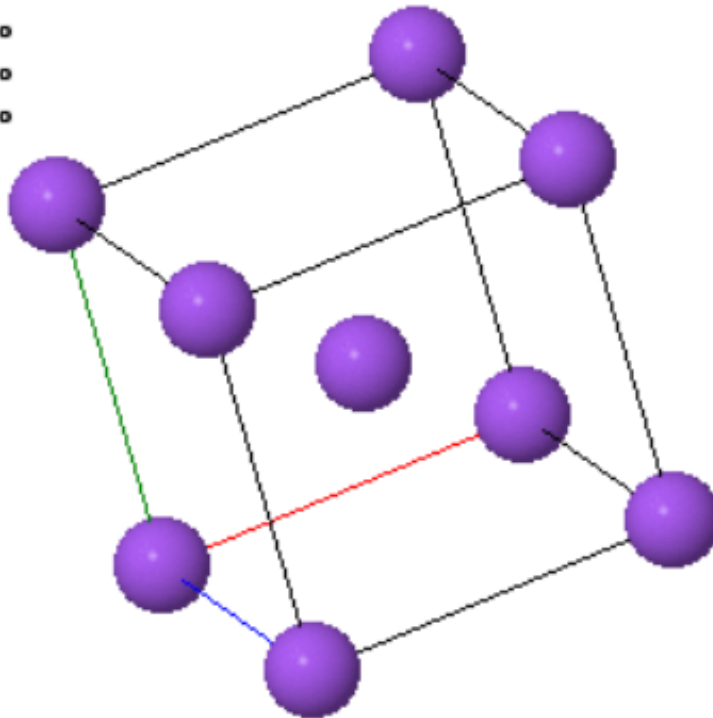
HCP = Hexagonal close pack ABAB...

Hexagonal Bravais lattice with two atoms in the basis.

body centered cubic bcc

W
Cr
Fe
Mo
Ta

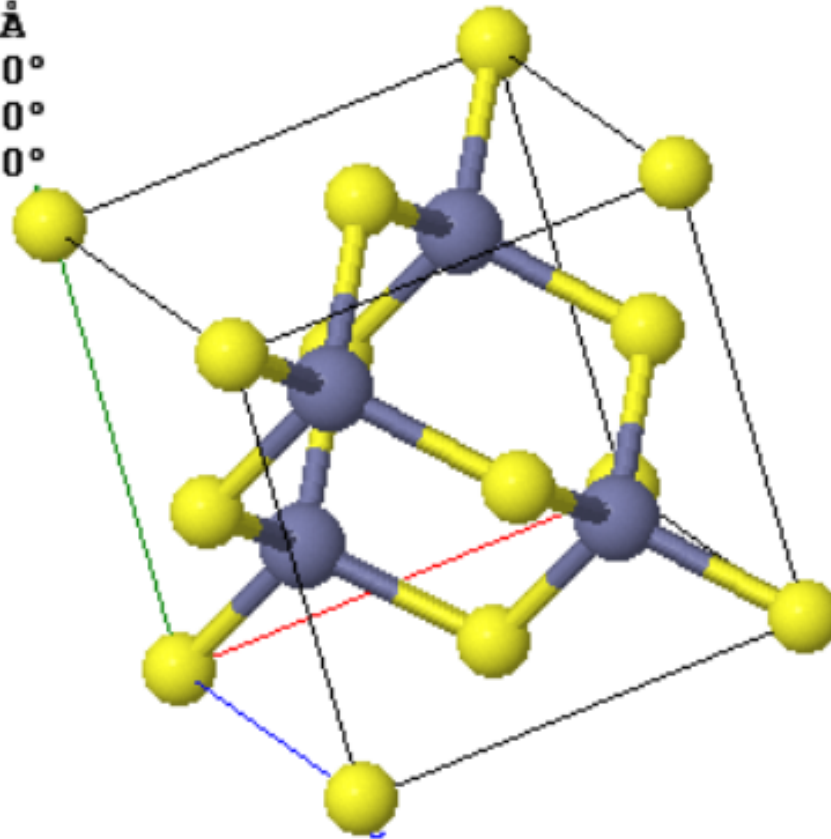
HM: IM-3M
a=4.291Å
b=4.291Å
c=4.291Å
α=90.000°
β=90.000°
γ=90.000°



zincblende

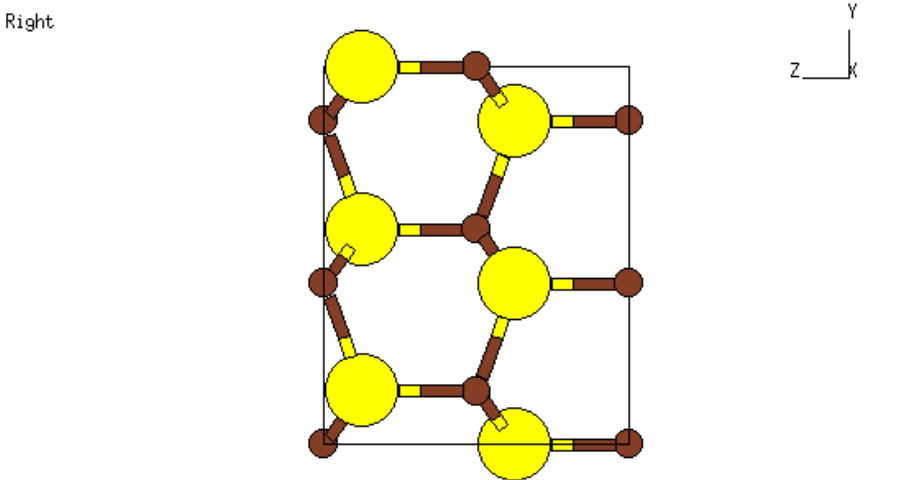
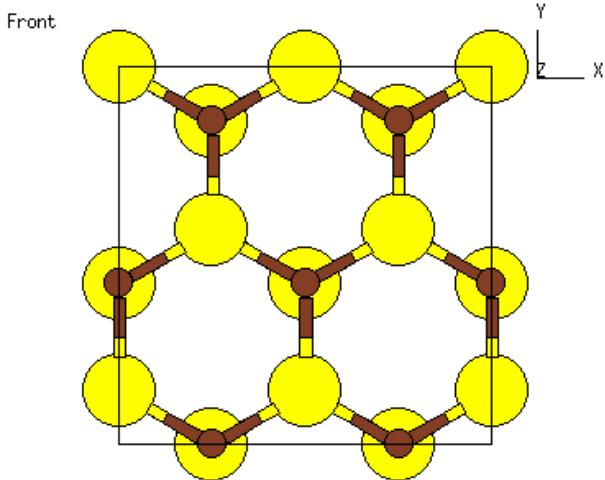
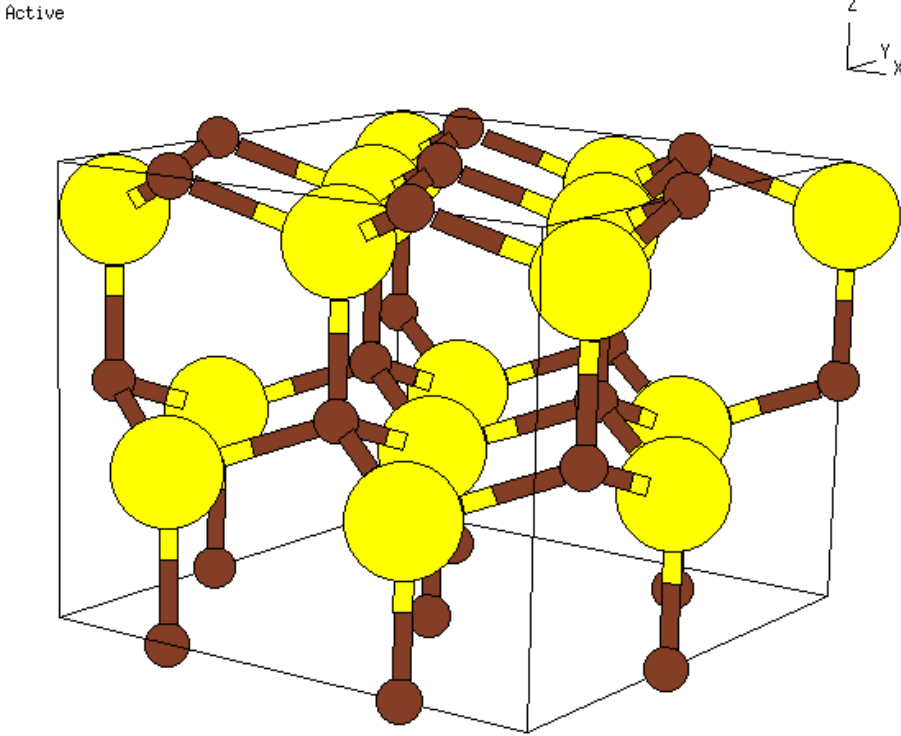
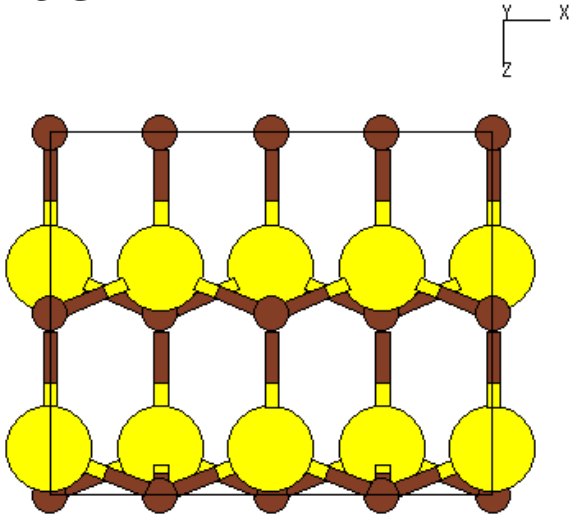
ZnS
GaAs
InP
GaP
InAs
AlAs

HM: F-43M
a=5.434Å
b=5.434Å
c=5.434Å
α=90.000°
β=90.000°
γ=90.000°

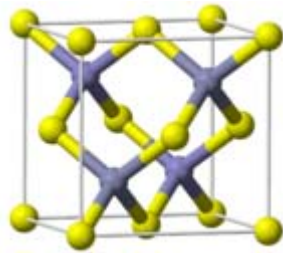


wurtzite

- ZnO
- CdS
- CdSe
- GaN
- AlN



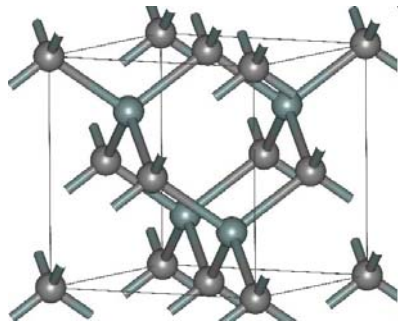
Structural phase transitions



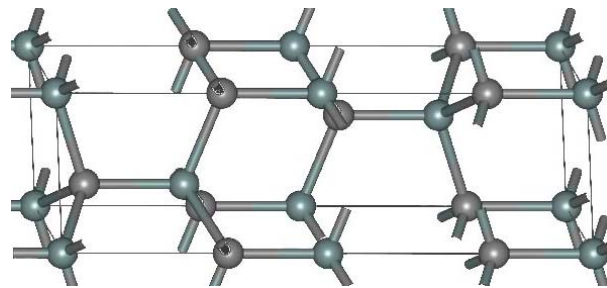
GaAs, Zinblende



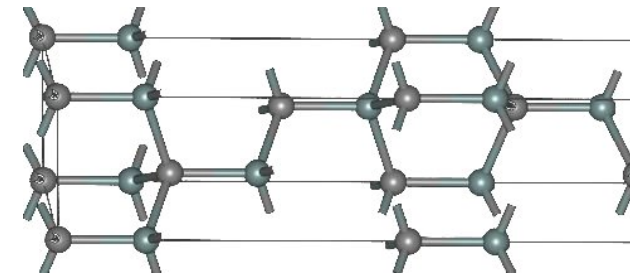
GaAs, Wurtzite



3C - SiC



4H - SiC



6H - SiC

SiC has about 100 polytypes