sp hybrid orbitals

The four orbitals are sp, sp, p, p

$$\psi_1 = \frac{1}{\sqrt{2}}\left(\phi_{2s} + \phi_{2p_z}\right) \qquad \psi_2 = \frac{1}{\sqrt{2}}\left(\phi_{2s} - \phi_{2p_z}\right)$$

$$\psi_3 = \phi_{2p_y} \qquad \psi_4 = \phi_{2p_z}$$

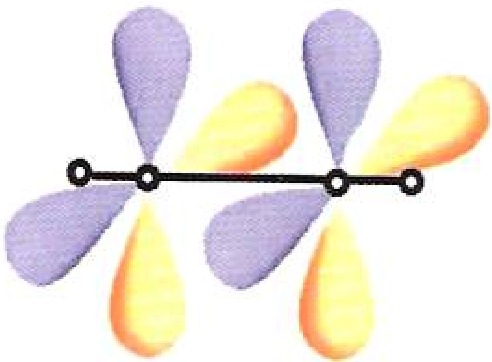
H — C ≡ C — H

s-sp

sp-sp, p-p, p-p

s-sp

acetylene



sp^2 hybrid orbitals   120^o

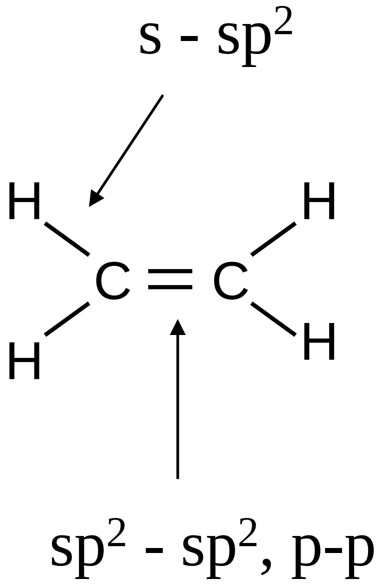
The four orbitals are sp^2,sp^2, sp^2, p

$$\psi_1 = \frac{1}{\sqrt{3}}\left(\phi_{2s} + \sqrt{2}\phi_{2p_x}\right)$$

$$\psi_2 = \frac{1}{\sqrt{3}}\phi_{2s} - \frac{1}{\sqrt{6}}\phi_{2p_x} + \frac{1}{\sqrt{2}}\phi_{2p_y}$$

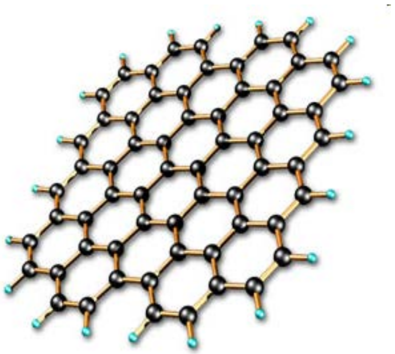
$$\psi_3 = \frac{1}{\sqrt{3}}\phi_{2s} - \frac{1}{\sqrt{6}}\phi_{2p_x} - \frac{1}{\sqrt{2}}\phi_{2p_y}$$

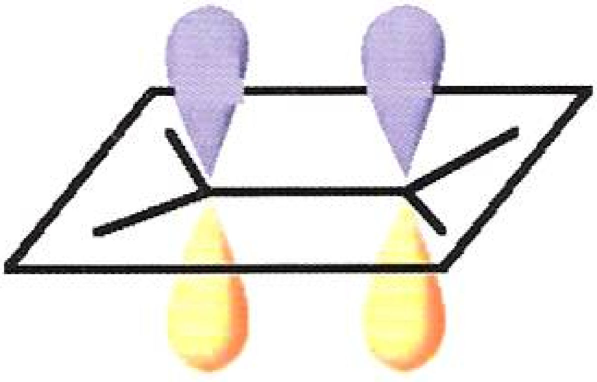
$$\psi_4 = \phi_{2p_z}$$



ethene

Graphene





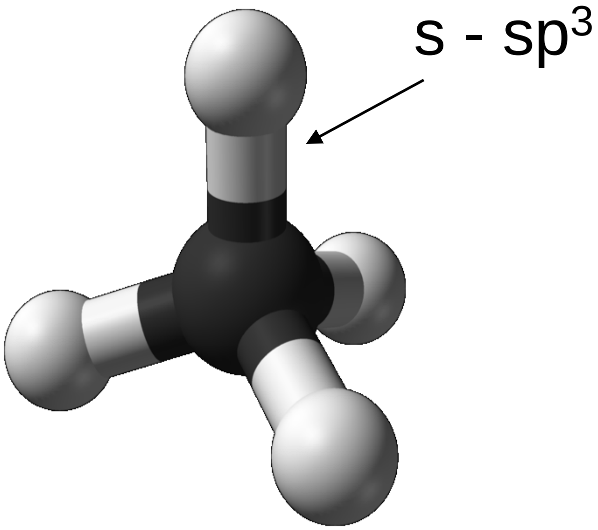
sp^3 hybrid orbitals 109^o

$$\psi_1 = \frac{1}{2}\left(\phi_{2s} + \phi_{2p_x} + \phi_{2p_y} + \phi_{2p_z}\right)$$

$$\psi_2 = \frac{1}{2}\left(\phi_{2s} + \phi_{2p_x} - \phi_{2p_y} - \phi_{2p_z}\right)$$

$$\psi_3 = \frac{1}{2}\left(\phi_{2s} - \phi_{2p_x} + \phi_{2p_y} - \phi_{2p_z}\right)$$

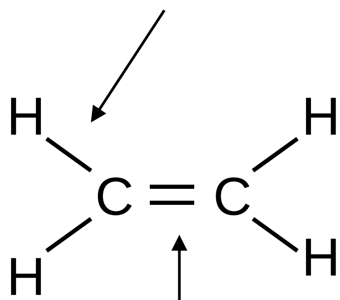
$$\psi_4 = \frac{1}{2}\left(\phi_{2s} - \phi_{2p_x} - \phi_{2p_y} + \phi_{2p_z}\right)$$



In this molecular orbital, the coefficients of these 4 atomic orbitals are about $c_{2s} = 1$, $c_{2px} = -1$, $c_{2py} = -1$, $c_{2pz} = 1$.

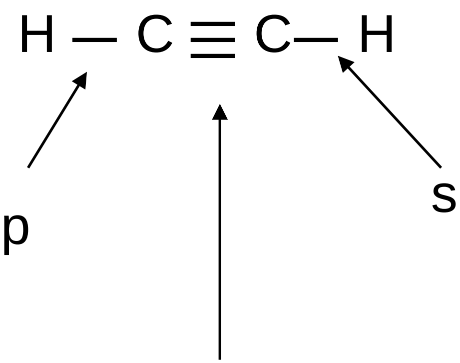
Examples of bonds

s - sp^2



ethene

sp^2 - sp^2, p-p

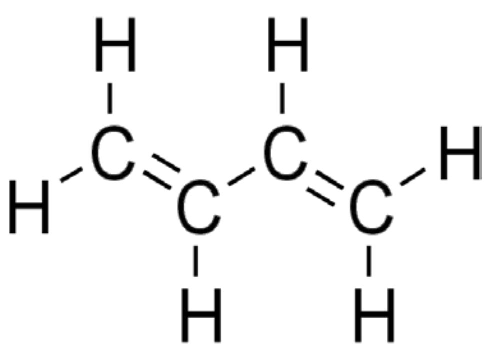


acetylene

s-sp

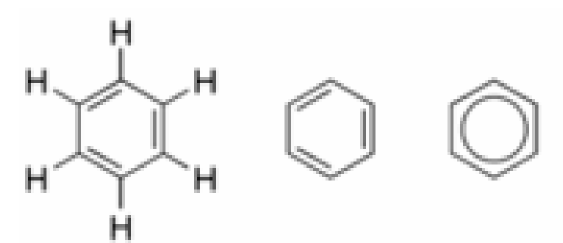
s-sp

sp-sp, p-p, p-p



butadiene

benzene



better described by molecular orbitals than by bonds

Symmetries

Molecules can be classified by their symmetries. The eigenfunctions of the Hamiltonian will also be eigenfunctions of the symmetry operators.

Symmetries belong to a group. for $A, B \in G, AB \in G$

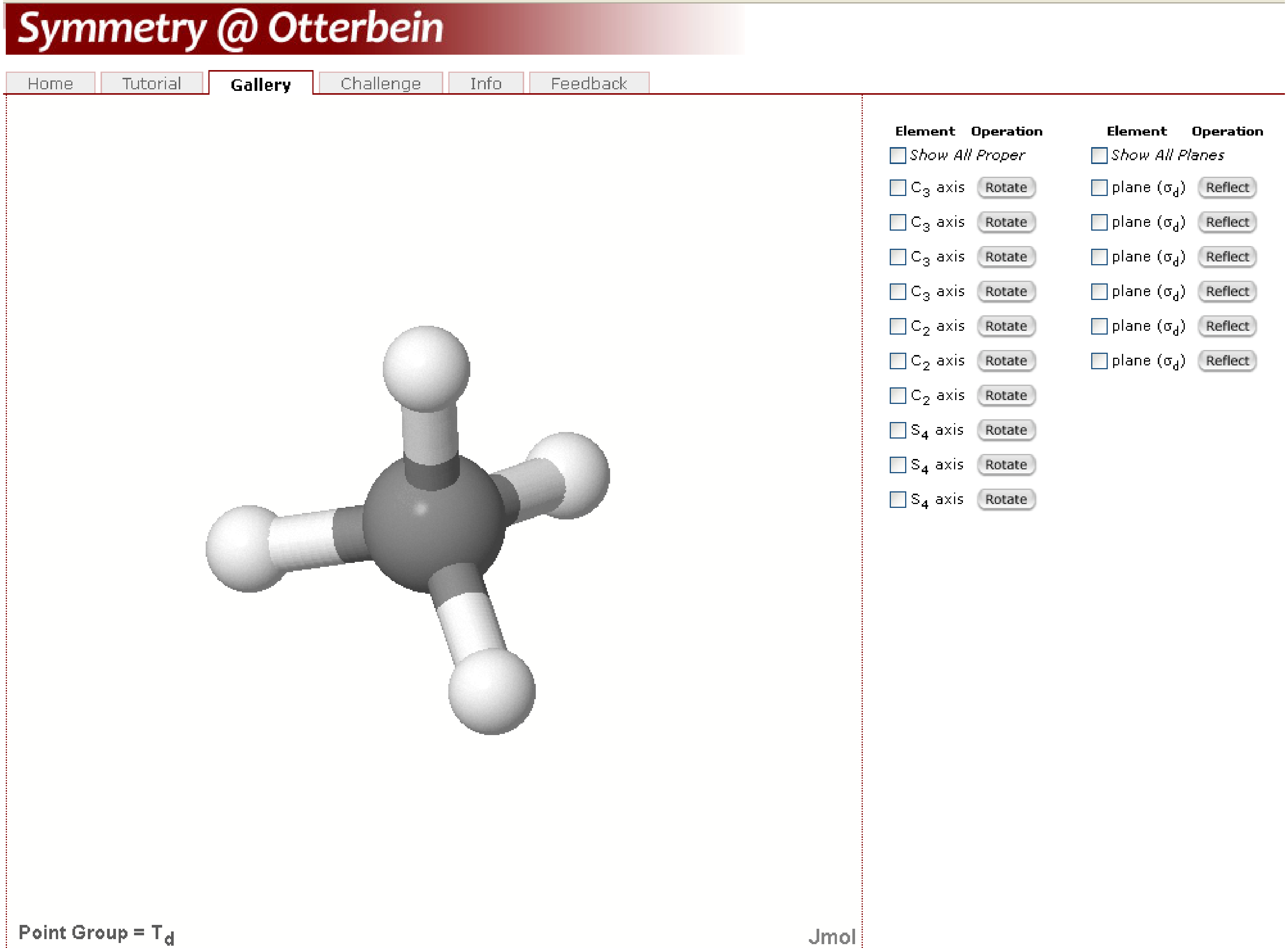
Point symmetries

If one point remains fixed during transformation, symmetries can be represented by 3×3 matrices.

$AB \in G$ for $A, B \in G$

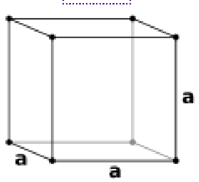
Rotation about the x axis by angle α:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



http://symmetry.otterbein.edu/gallery/index.html

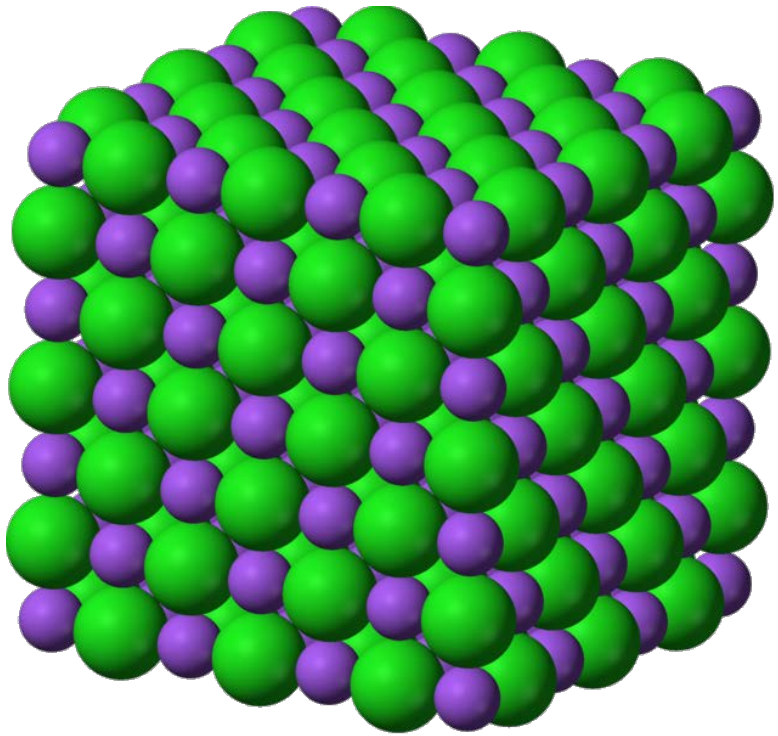
The 32 Crystal Classes

Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Cubic 	tetrahedral	23	T	195-199	3	4	-	-	-	n		12
	diploidal	$m3$	T_h	200-206	3	4	-	-	3	y		24
	gyroidal	432	O	207-214	6	4	3	-	-	n		24
	hextetrahedral	$\bar{4}3m$	T_d	215-220	3	4	-	-	6	n	216: Zincblende, ZnS, GaAs, GaP, InAs, SiC	24
	hexoctahedral	$m3m$	O_h	221-230	6	4	3	-	9	y	221: CsCl, cubic perovskite 225: fcc, Al, Cu, Ni, Ag, Pt, Au, Pb, γ-Fe, NaCl 227: diamond, C, Si, Ge, α-Sn, spinel 229: bcc, Na, K, Cr, α-Fe, β-Ti, Nb, Mo, Ta	48

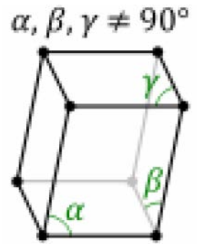
http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html

Crystal structure

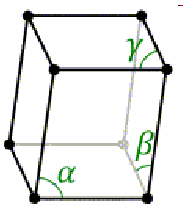
A crystal is a three dimensional periodic arrangement of atoms.



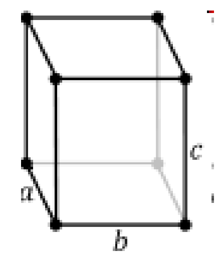
7 Crystal Systems



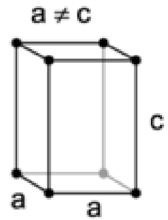
triclinic: a ≠ b ≠ c and α ≠ β ≠ γ ≠ 90°



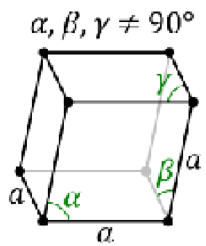
monoclinic: a ≠ b ≠ c and α ≠ 90° β = γ = 90°



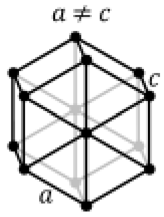
orthorhombic: a ≠ b ≠ c and α = β = γ = 90°



tetragonal: a = b ≠ c and α = β = γ = 90°

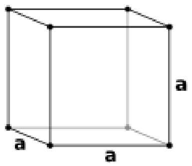


rhombohedral: a = b = c and α ≠ β ≠ γ ≠ 90°



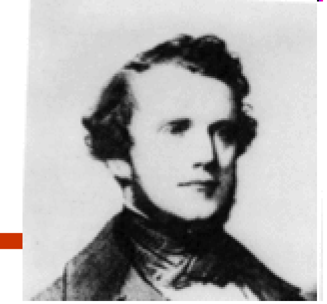
hexagonal: a = b ≠ c and α = β = 90°, γ =120°

cubic a = b = c and α = β = γ = 90°

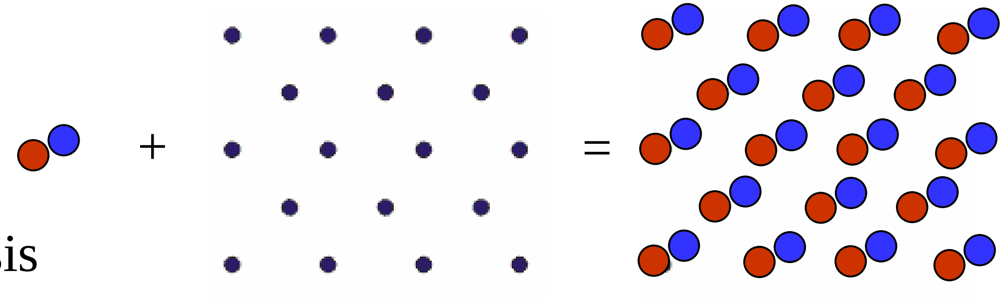


α is the angle between b and c

Bravais lattice



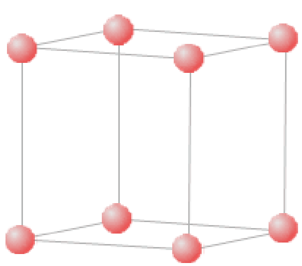
Auguste Bravais



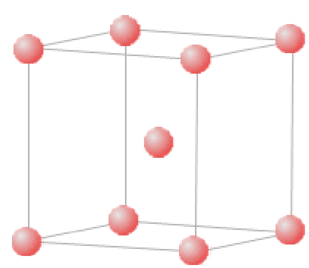
basis

Bravais lattice

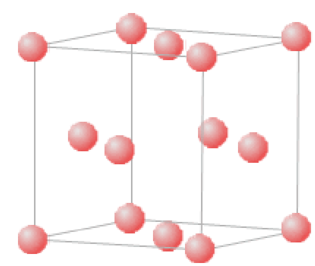
Crystal



simple cubic

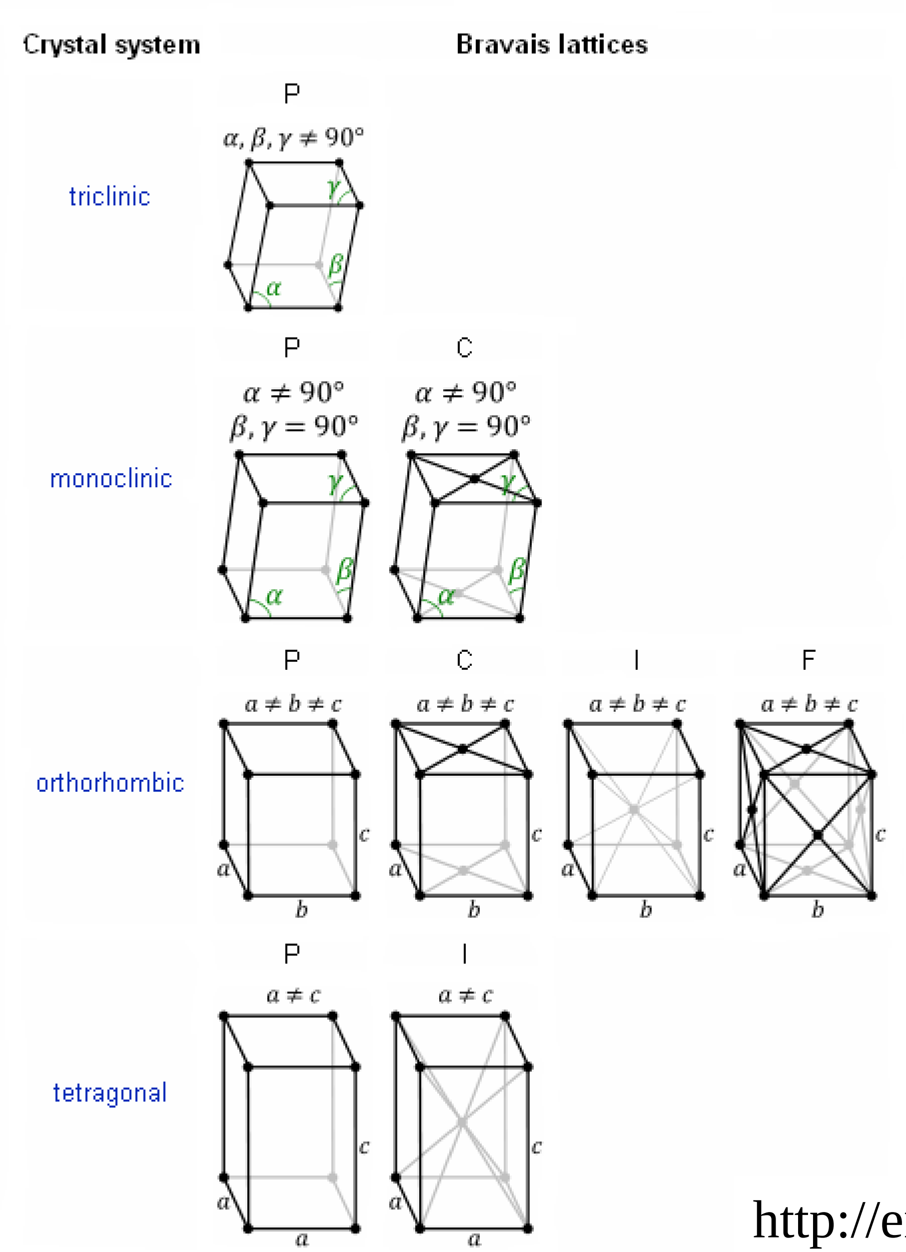


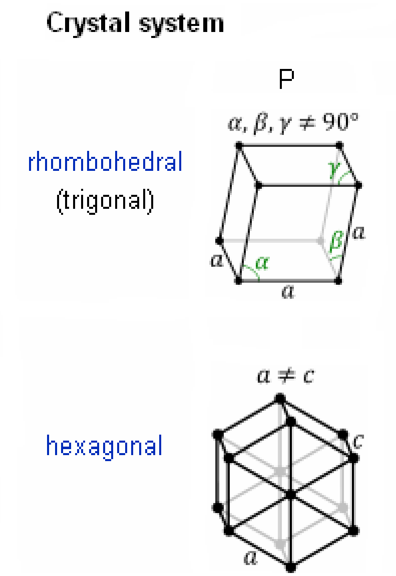
body centered cubic, bcc



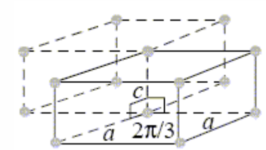
face centered cubic, fcc

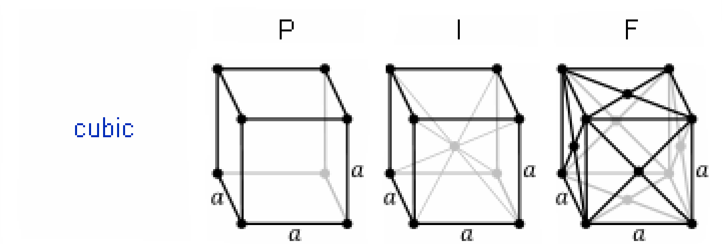
14 Bravais lattices





Points of a Bravais lattice do not necessarily represent atoms.





P … primitive
I … body centered
F … face centered
C … centered

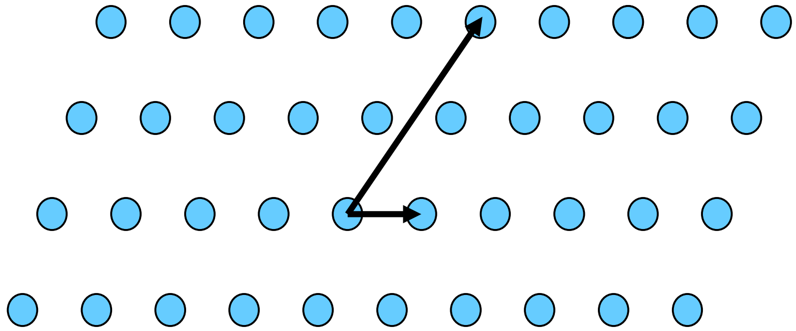
http://en.wikipedia.org/wiki/Bravais_lattice

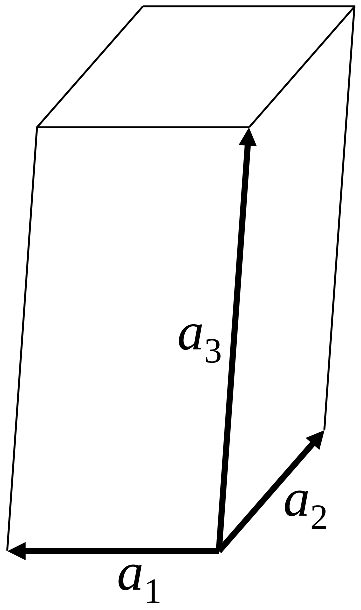
Primitive lattice vectors

Every point of a Bravais lattice can be reached from another point on the lattice by a translation vector

Translation vector

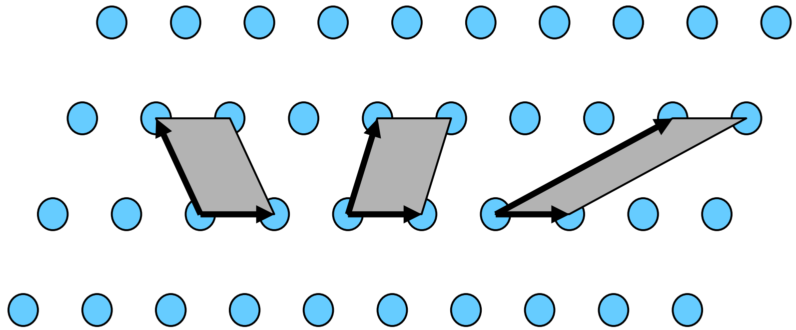
$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 = \cdots -2, -1, 0, 1, 2, \cdots$$



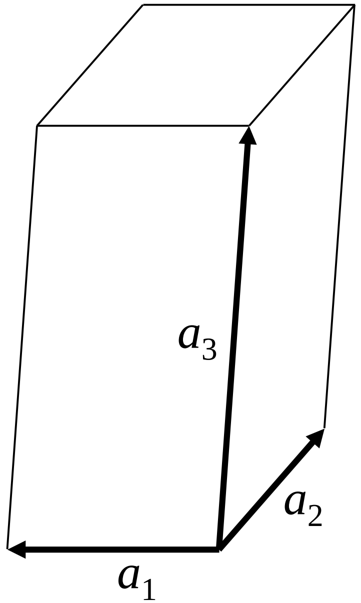


Primitive lattice vectors

Primitive Unit Cell



There is more than one choice for a primitive unit cell



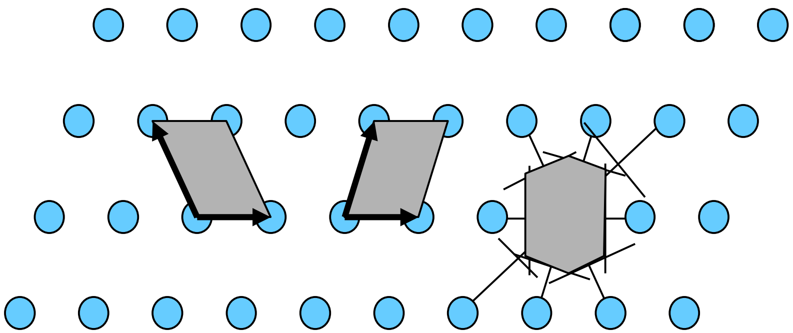
volume of a unit cell =

$$\left| \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 \right|$$

$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 = \cdots -2, -1, 0, 1, 2, \cdots$$

Unit Cells

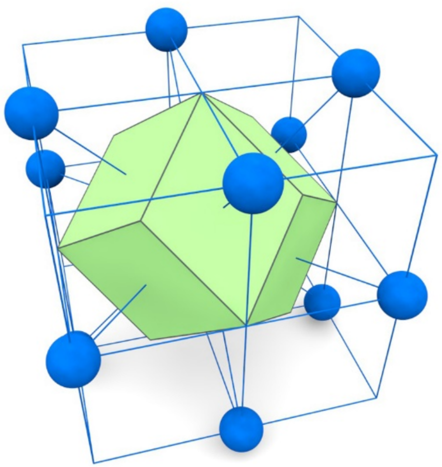
There is more than one choice for a primitive unit cell



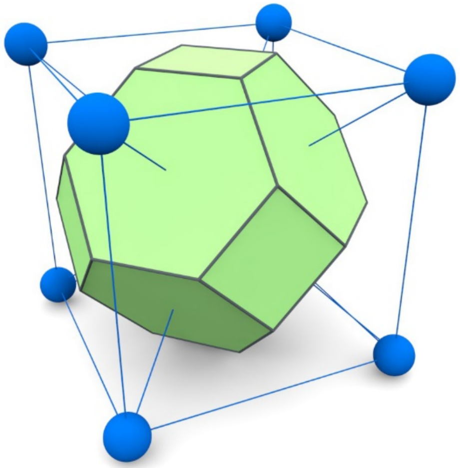
Eugene Wigner

Frederick Seitz

Wigner-Seitz primitive unit cell



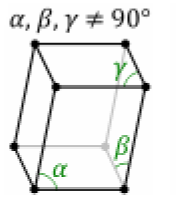
fcc



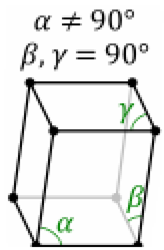
bcc

Conventional (crystallographic) unit cell

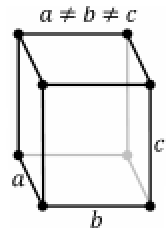
triclinic



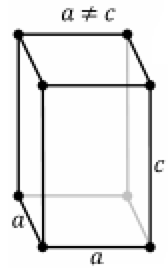
monoclinic



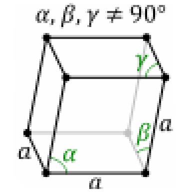
orthorhombic



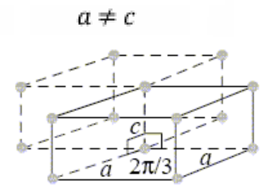
tetragonal



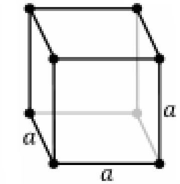
rhombohedral
(trigonal)



hexagonal



cubic

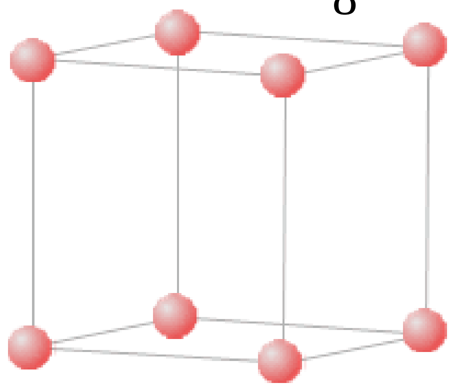


6 faces, 8 corners

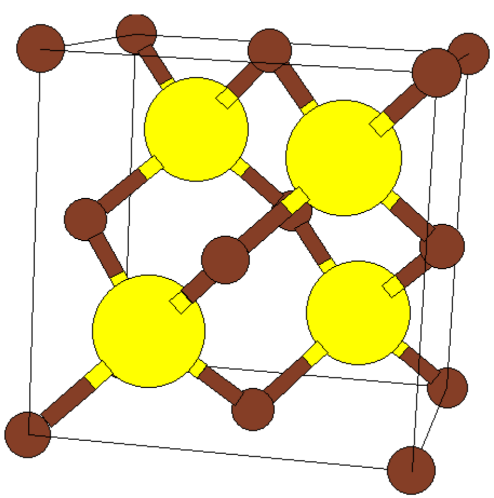
http://en.wikipedia.org/wiki/Bravais_lattice

Conventional (crystalographic) unit cell

$$8\times\frac{1}{8}=1$$

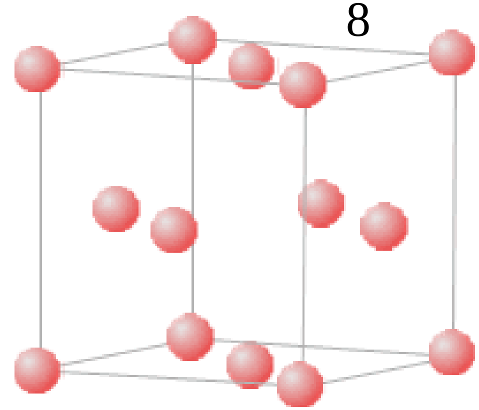


simple cubic



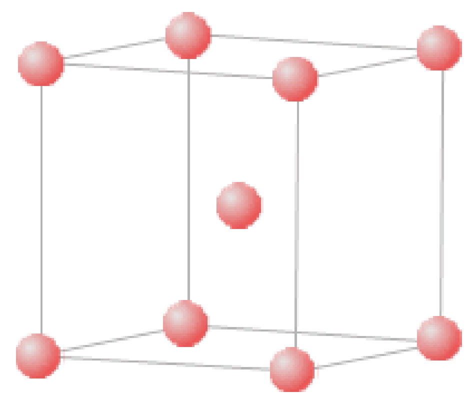
zincblende

$$8\times\frac{1}{8}+6\times\frac{1}{2}=4$$



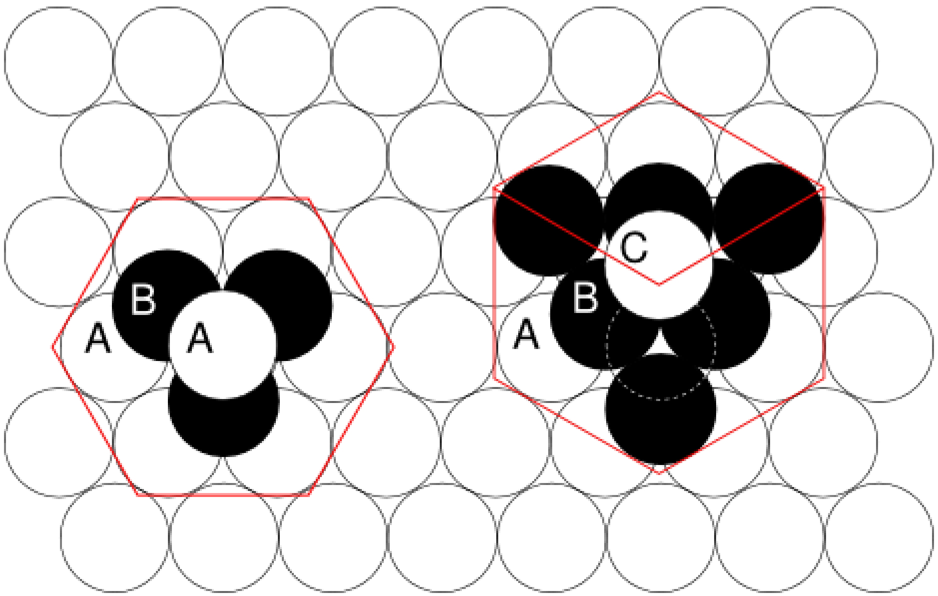
fcc

$$8\times\frac{1}{8}+1=2$$

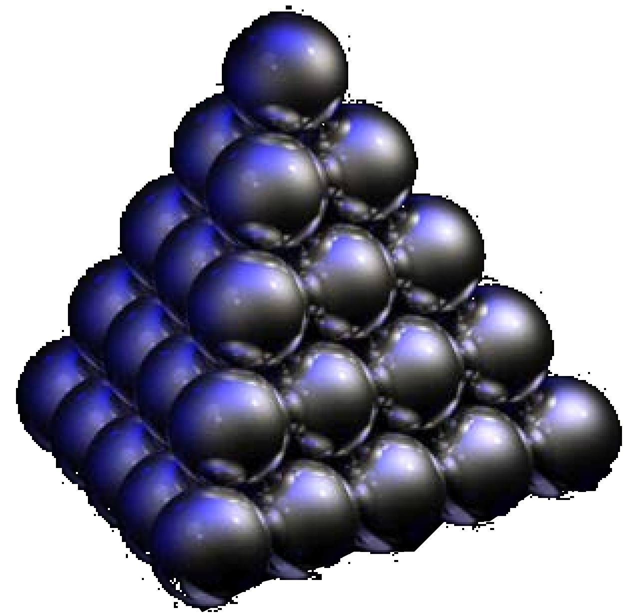


bcc

Close packing



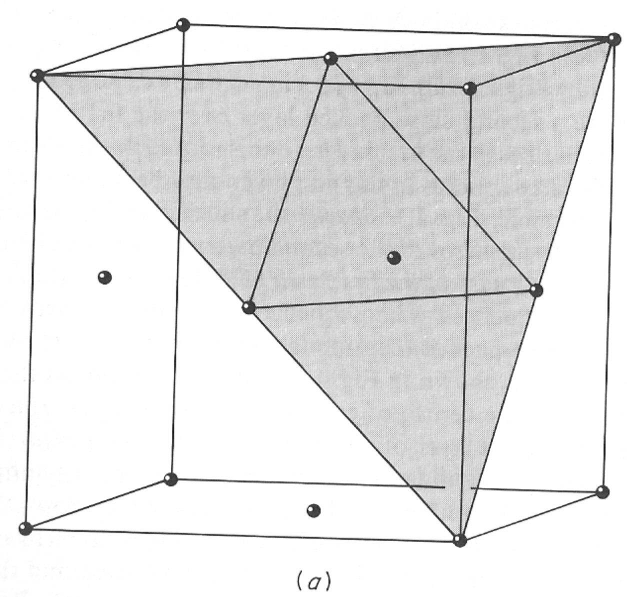
HCP FCC



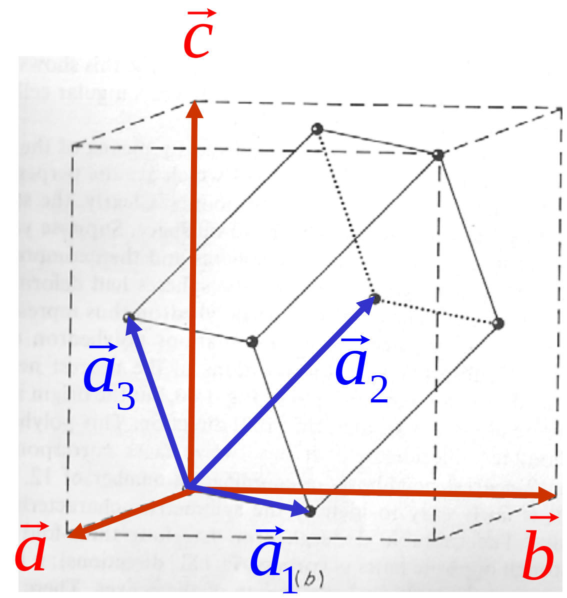
HCP = Hexagonal close pack

Hexagonal Bravais lattice with two atoms in the basis.

Fcc

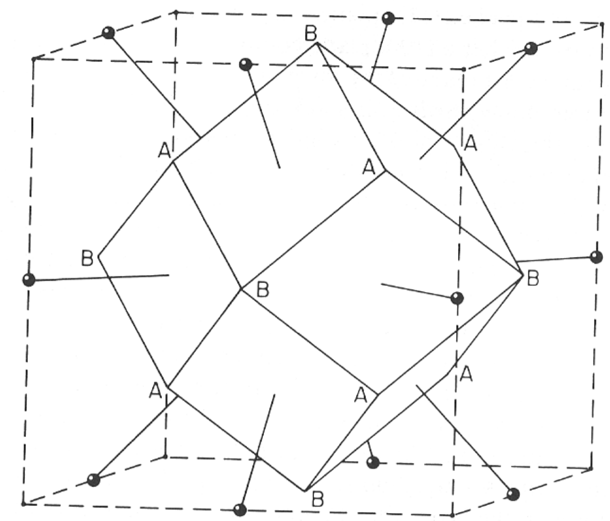


Crystalographic unit cell showing close packed plane



Crystalographic lattice vectors

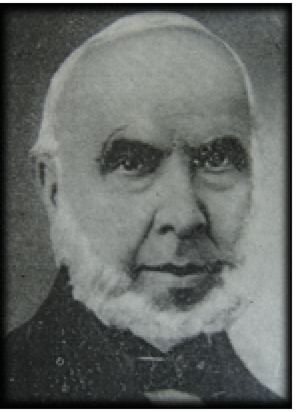
Primitive lattice vectors



Wigner-Seitz cell

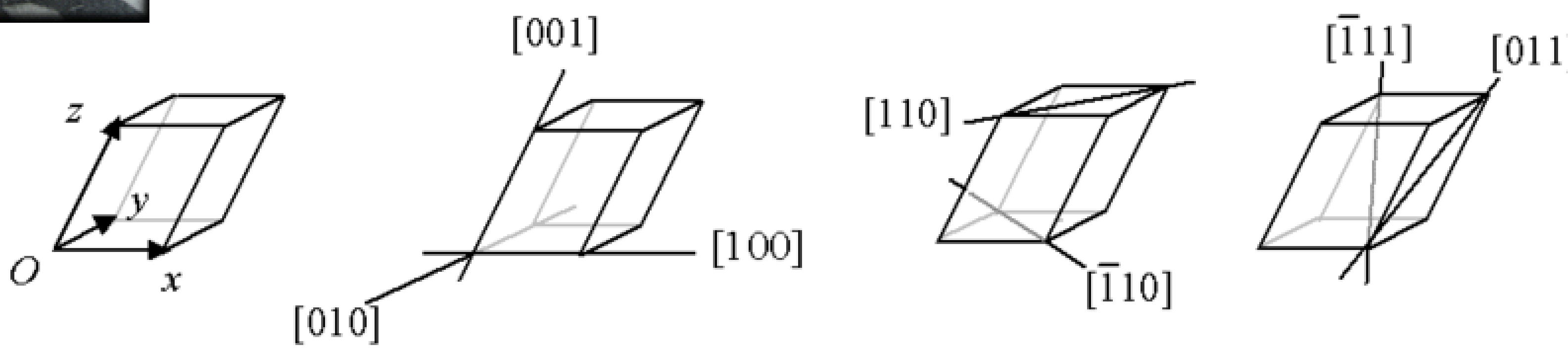
From: Hall, Solid State Physics

Miller indices: Crystal direction [*uvw*]



[*uvw*] = vector in direction $u\,\mathbf{a} + v\,\mathbf{b} + w\,\mathbf{c}$

lattice vectors of the crystallographic unit cell

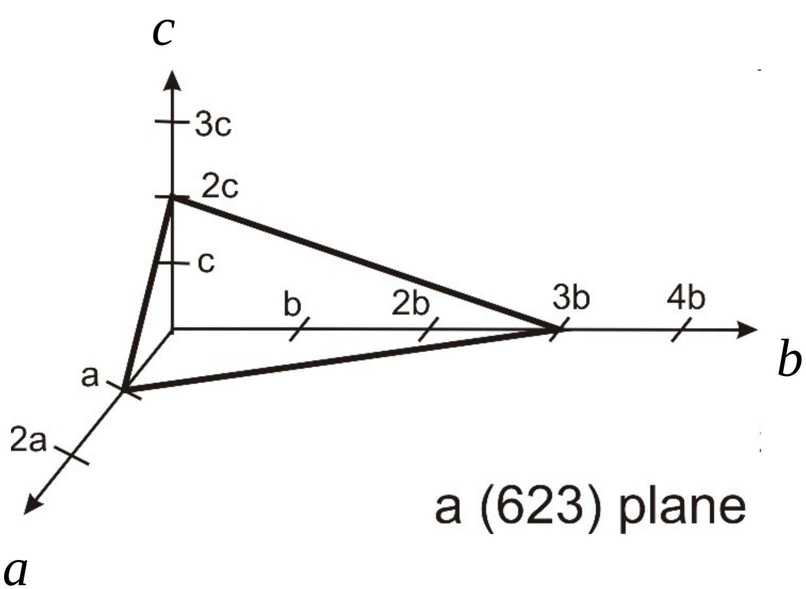


notation: $-1 = \bar{1}$

[ ] specific direction

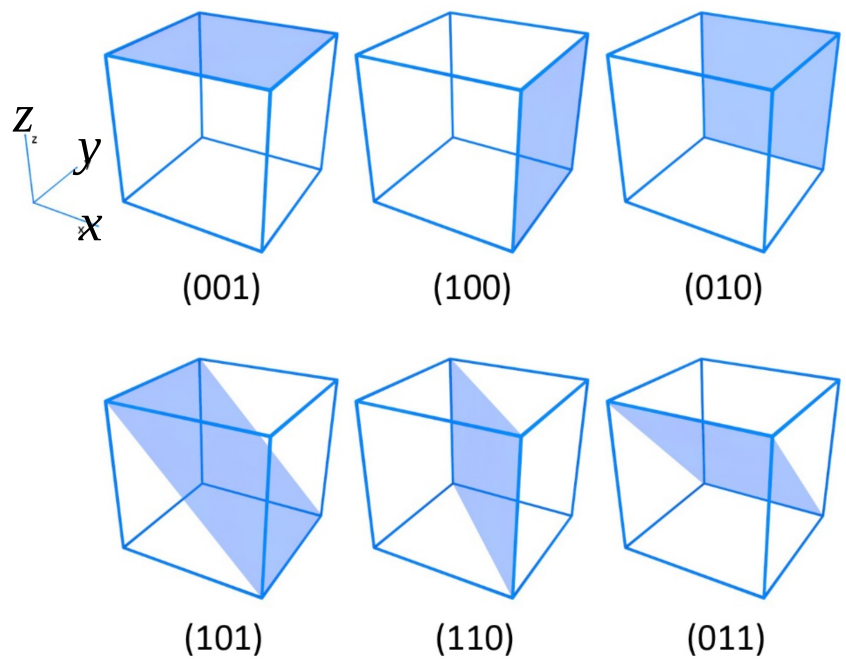
< > family of equivalent directions

Miller indices: Crystal planes



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

always use integers for h,k,l

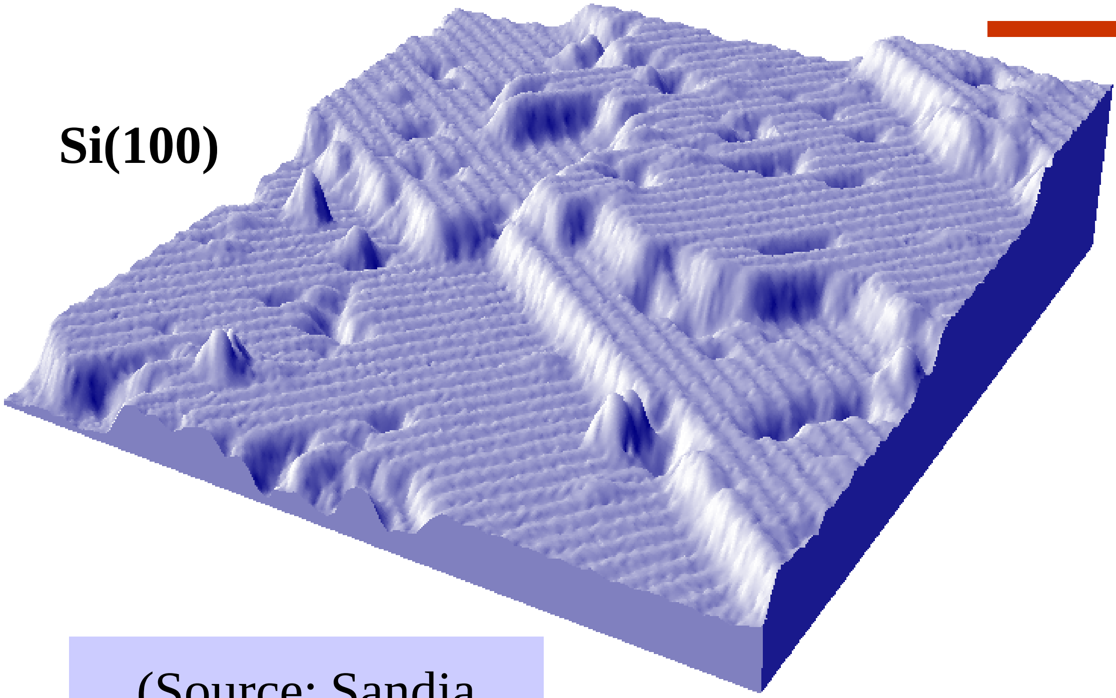


( ) specific plane
{ } family of equivalent planes

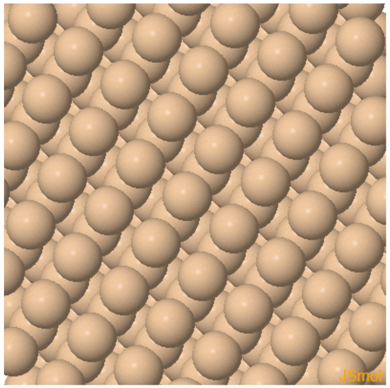
MOSFETs are made on <100> wafers

Silicon surfaces

Si(100)



(Source: Sandia Nat.Labs.)



Si(111)