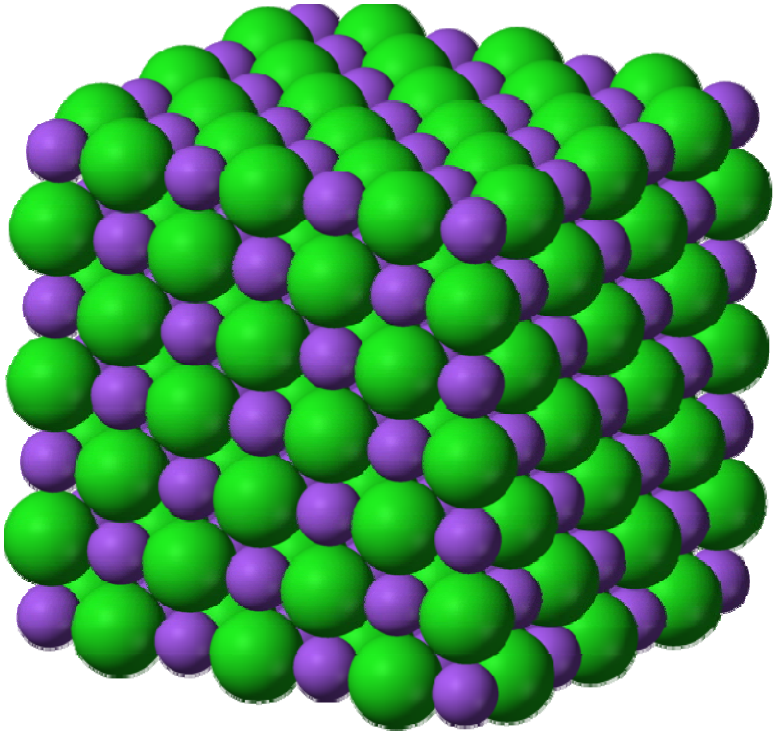
6. Crystal structure

March 22, 2018

Crystal structure

A crystal is a three dimensional periodic arrangement of atoms.



7 Crystal Systems

triclinic: a ≠ b ≠ c and $\alpha \neq \beta \neq \gamma \neq 90°$

monoclinic: a ≠ b ≠ c and $\alpha \neq 90° \ \beta = \gamma = 90°$

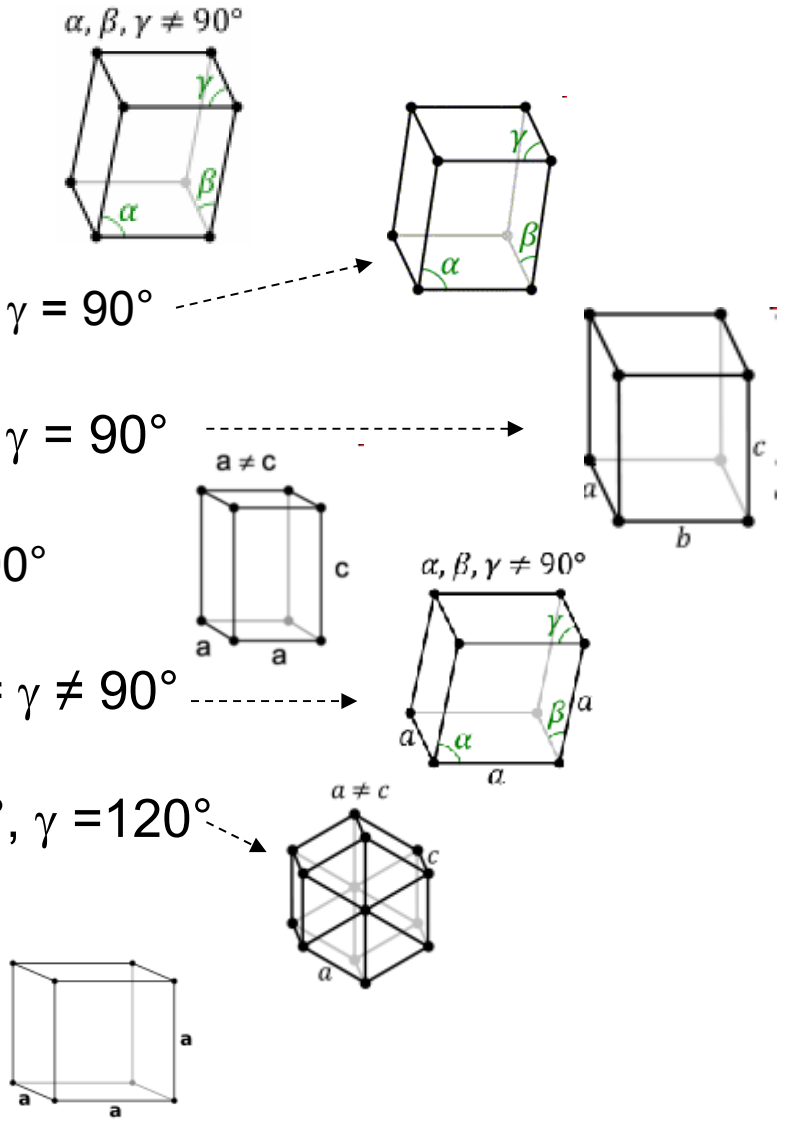
orthorhombic: a ≠ b ≠ c and $\alpha = \beta = \gamma = 90°$

tetragonal: a = b ≠ c and $\alpha = \beta = \gamma = 90°$

rhombohedral: a = b = c and $\alpha \neq \beta \neq \gamma \neq 90°$

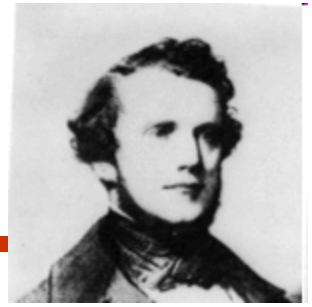
hexagonal: a = b ≠ c and $\alpha = \beta = 90°, \gamma = 120°$

cubic a = b = c and $\alpha = \beta = \gamma = 90°$

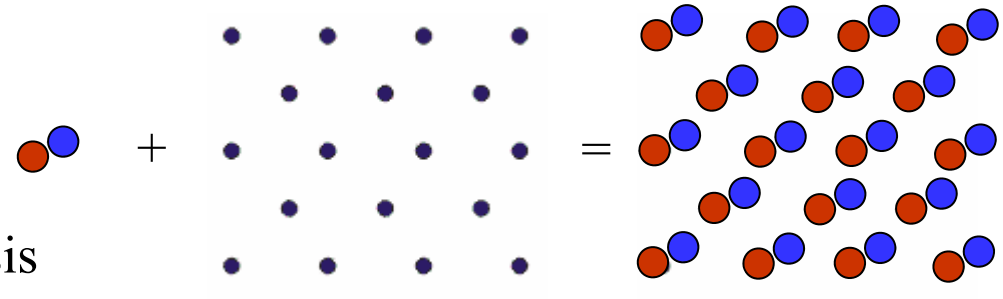


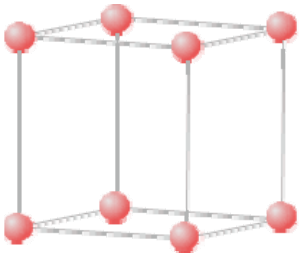
α is the angle between b and c

Bravais lattice

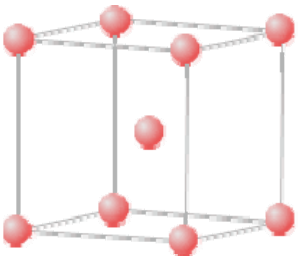


Auguste Bravais

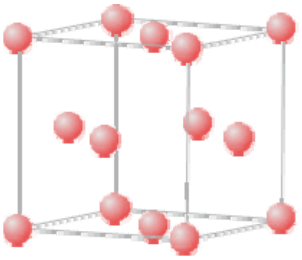




simple cubic

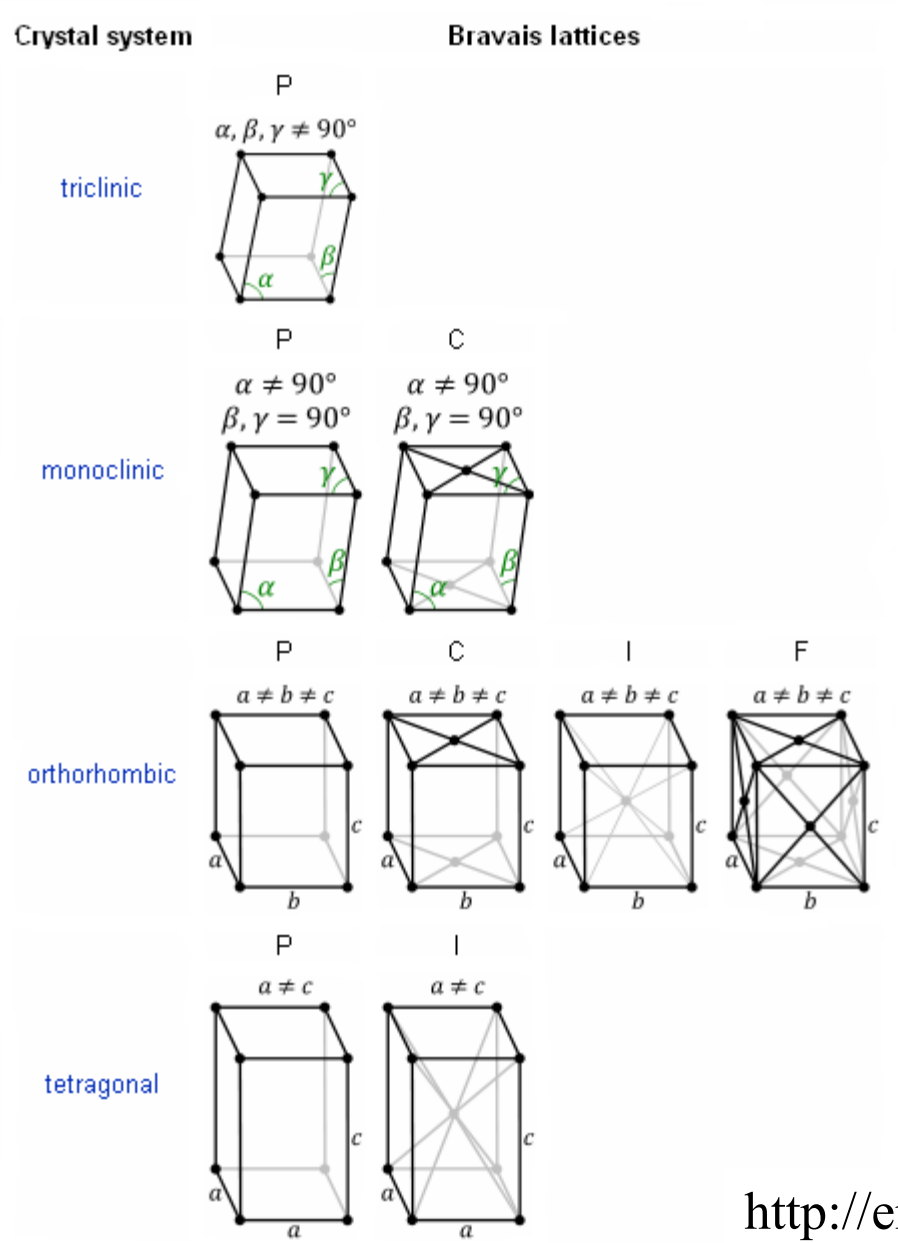


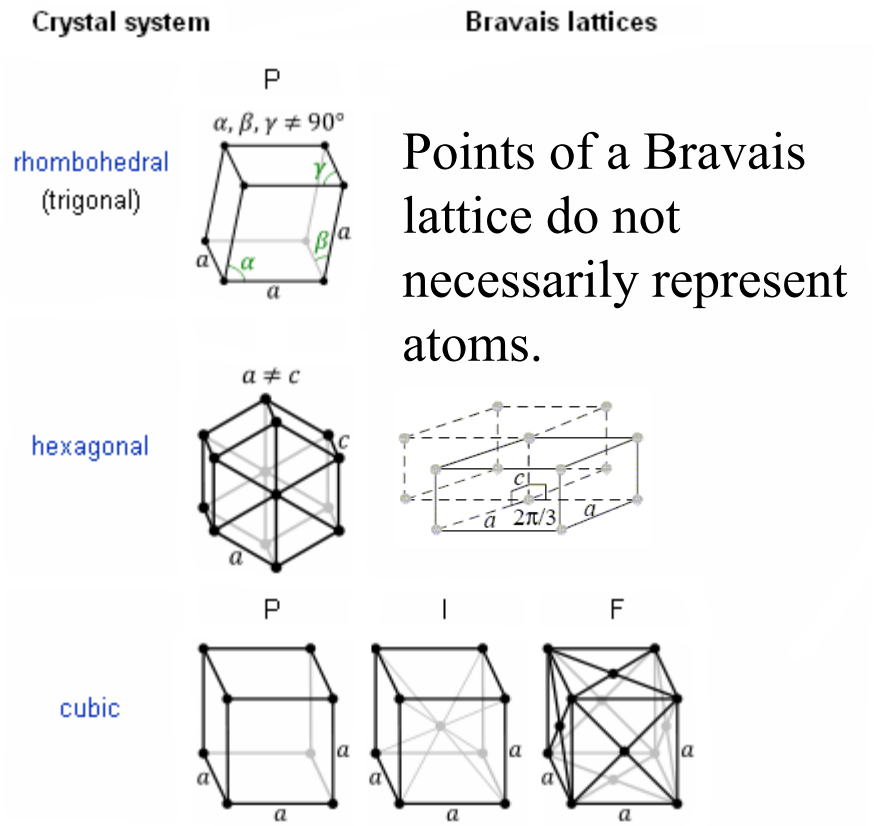
body centered cubic, bcc



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

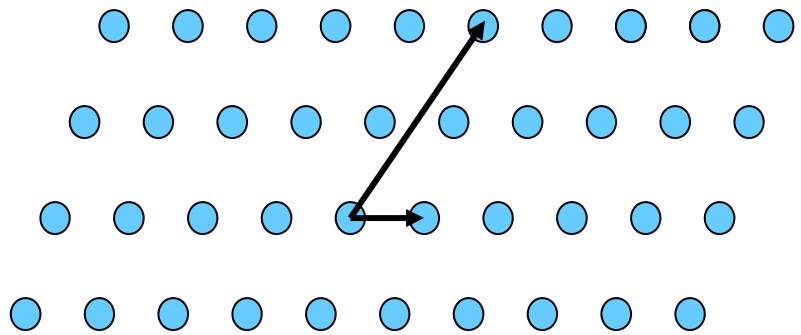
http://en.wikipedia.org/wiki/Bravais_lattice

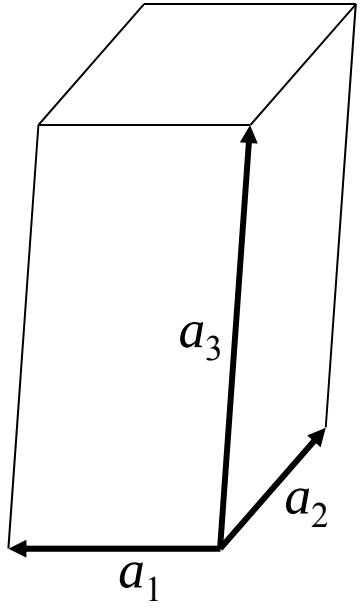
Primitive lattice vectors

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

Translation vector

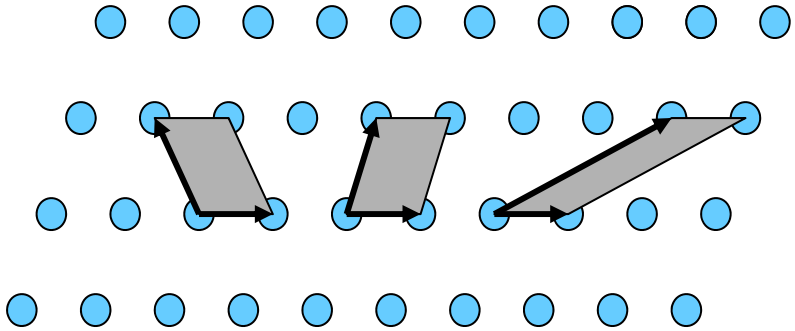
$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 = \cdots -2, -1, 0, 1, 2, \cdots$$



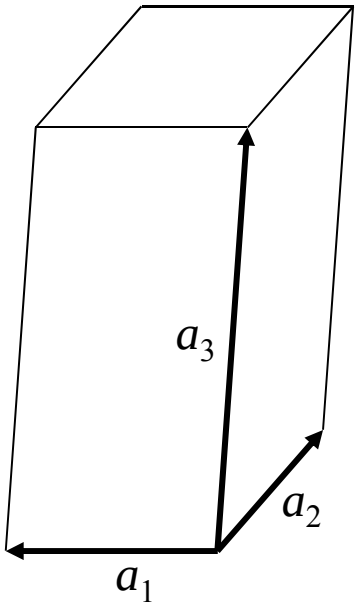


Primitive lattice vectors

Primitive Unit Cell



There is more than one choice for a primitive unit cell



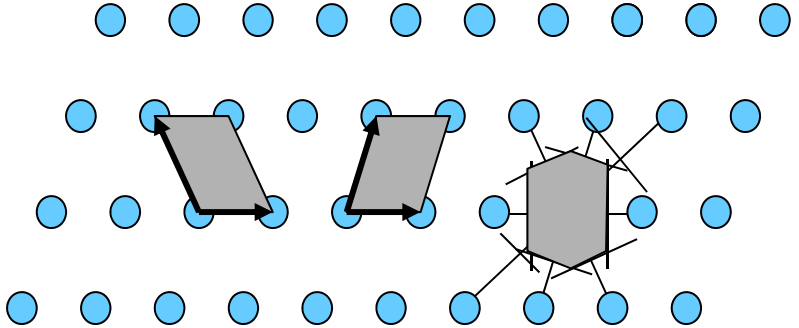
volume of a unit cell =

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

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

Unit Cells

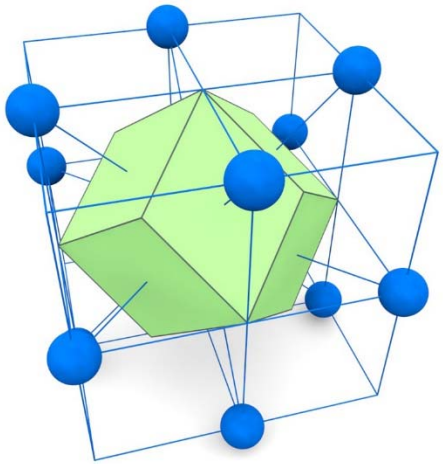
There is more than one choice for a primitive unit cell



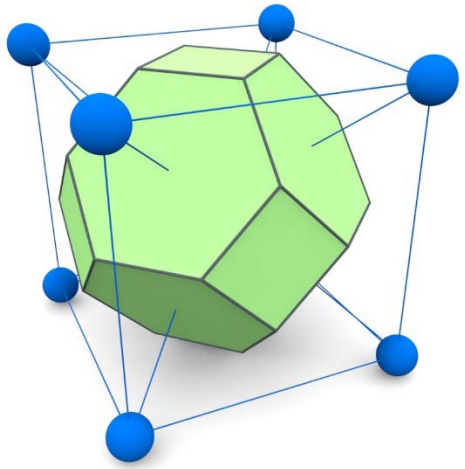
Eugene Wigner

Frederick Seitz

Wigner-Seitz primitive unit cell



fcc



bcc

Wigner-Seitz cells

The set of planes perpendicular to a vector $A_x\hat{x} + A_y\hat{y} + A_z\hat{z}$ is,

$$A_x x + A_y y + A_z z = C,$$

where C is any constant. If a point (x_0, y_0, z_0) on the plane is known, C can be calculated,

$$C = A_x x_0 + A_y y_0 + A_z z_0.$$

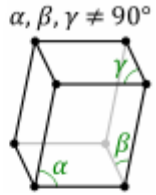
The app below will solve 3 linear equations for three unknowns. (It determines the point where three planes intersect.)

7	$x+$	3	$y+$	2	$z =$	6
5	$x+$	9	$y+$	4	$z =$	6
2	$x+$	1	$y+$	8	$z =$	2

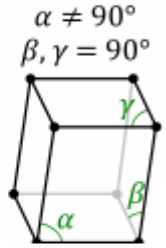
solve

Conventional (crystallographic) unit cell

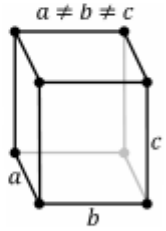
triclinic



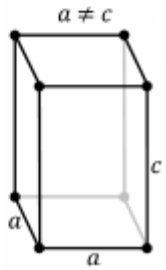
monoclinic



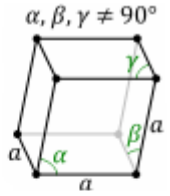
orthorhombic



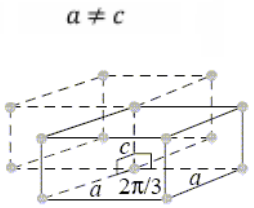
tetragonal



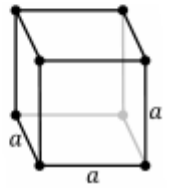
rhombohedral (trigonal)



hexagonal



cubic



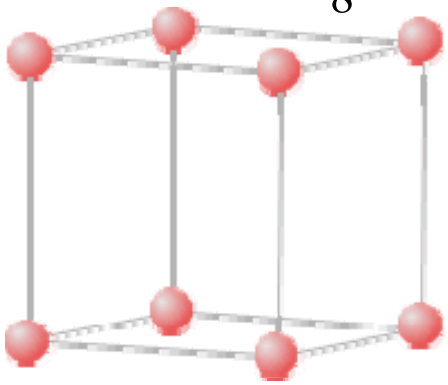
α is the angle between *b* and *c*
β is the angle between *a* and *c*
γ is the angle between *a* and *b*

6 faces, 8 corners

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

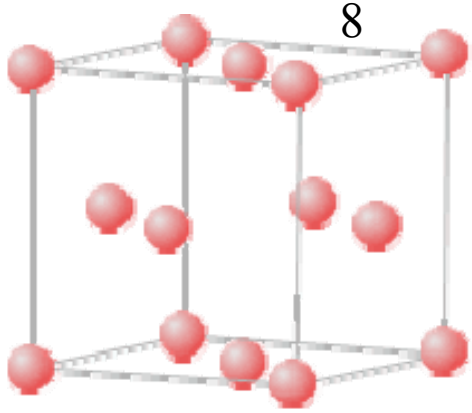
Conventional (crystalographic) unit cell

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

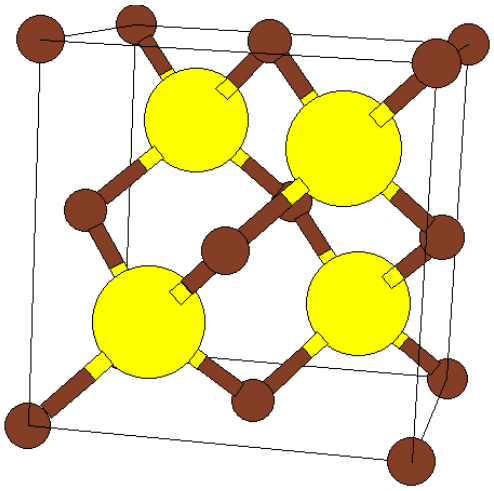


simple cubic

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

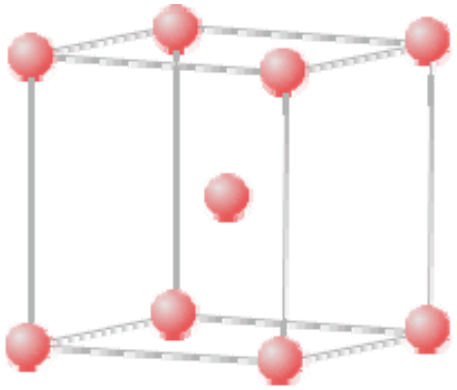


fcc



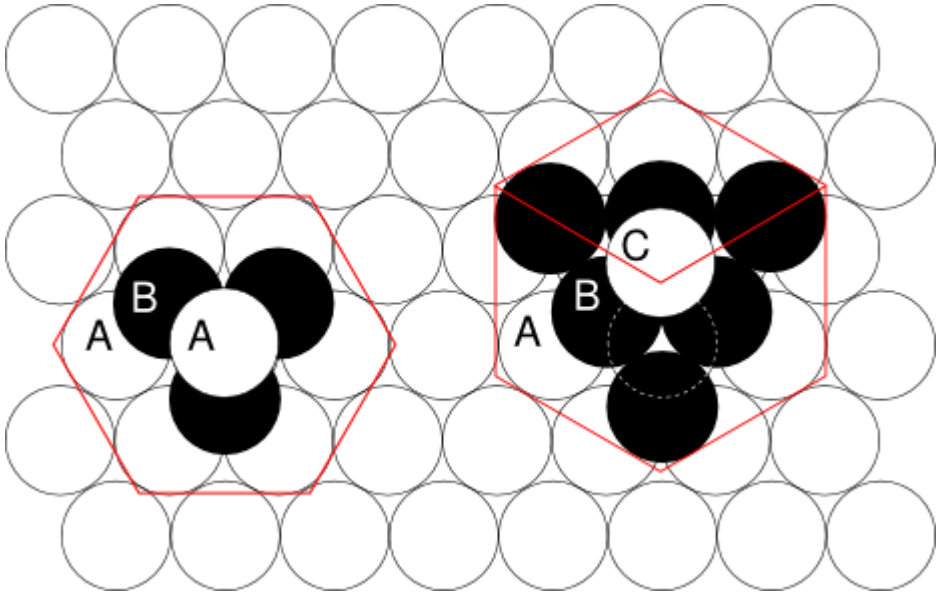
zincblende

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

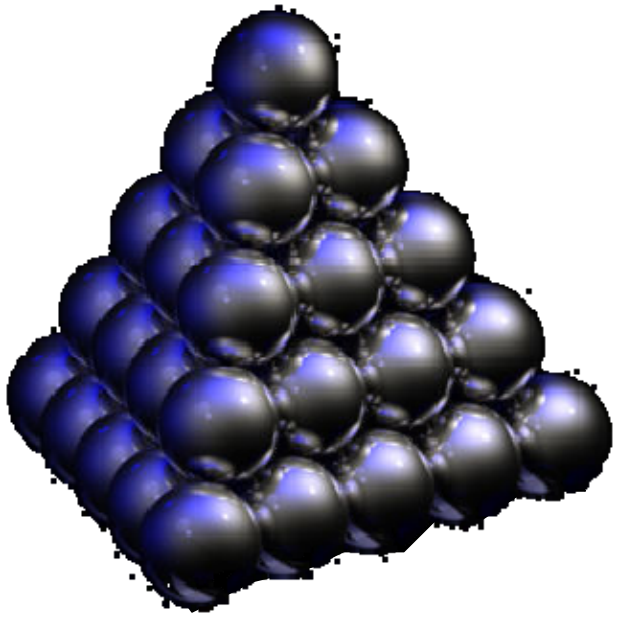


bcc

Close packing

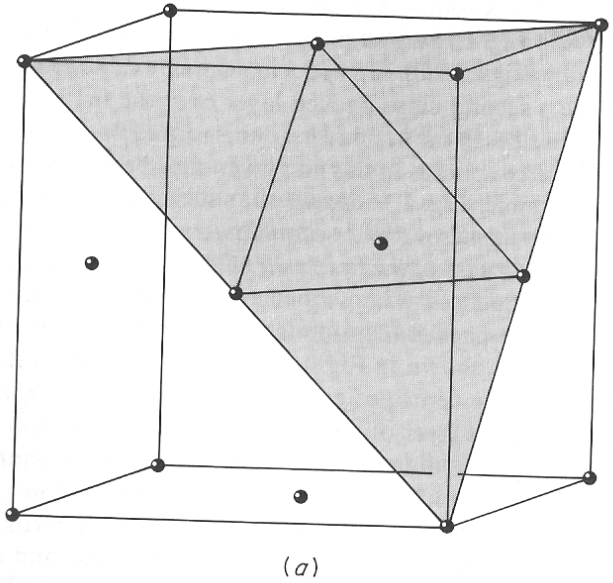


HCP FCC

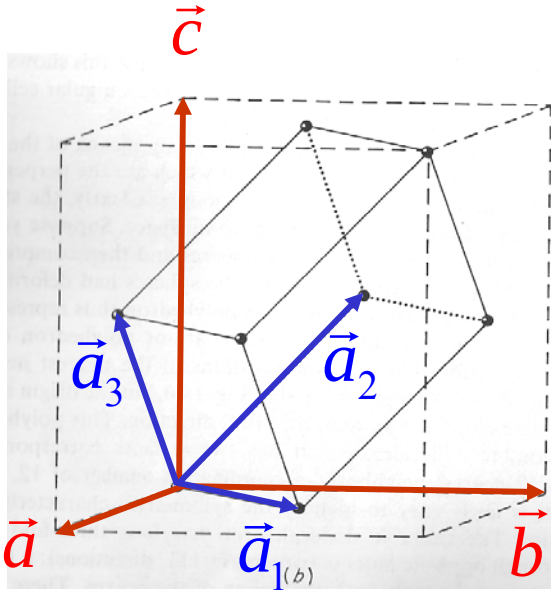


HCP = Hexagonal close pack
Hexagonal Bravais lattice with two atoms in the basis.

Fcc

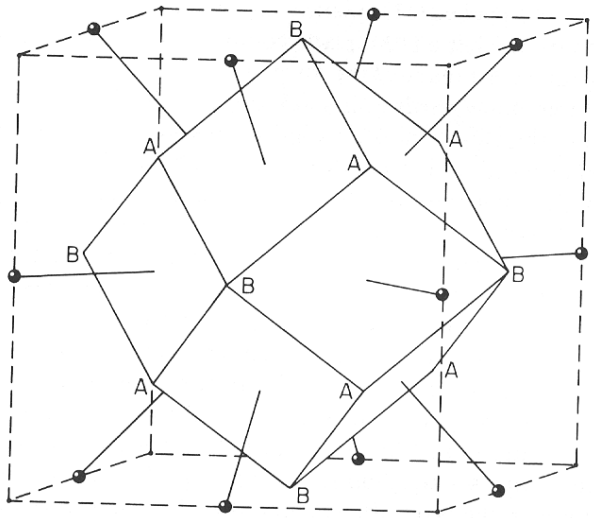


Crystalographic unit cell showing close packed plane



Crystalographic lattice vectors

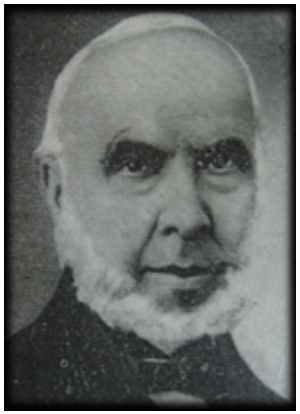
Primitive lattice vectors



Wigner-Seitz cell

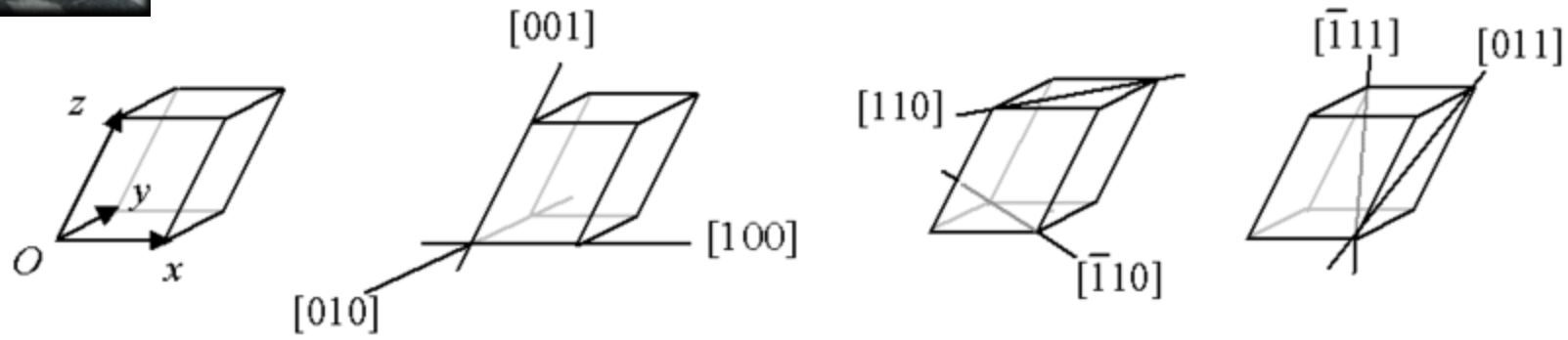
From: Hall, Solid State Physics

Miller indices: Crystal direction [*uvw*]



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

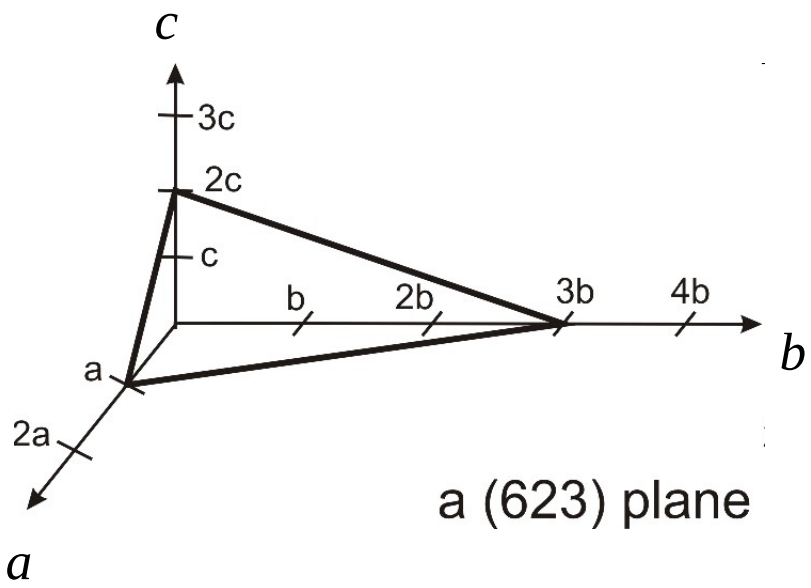
lattice vectors of the crystallographic unit cell



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

[ ] specific direction
< > family of equivalent directions

Miller indices: Crystal planes



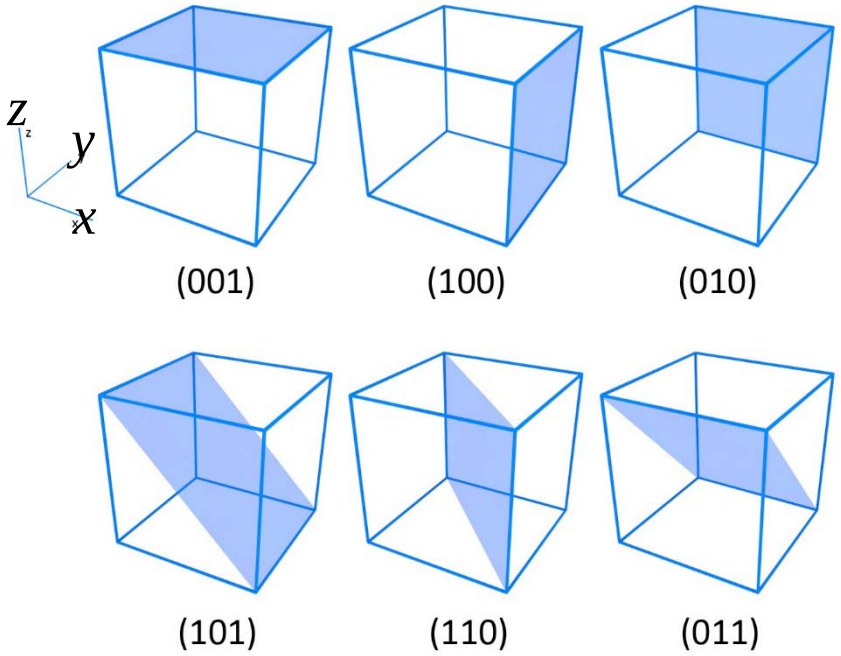
A plane with the intercepts $1/h, 1/k, 1/l$ is the (h,k,l) plane.

always use integers for h,k,l

( ) specific plane

{ } family of equivalent planes

MOSFETs are made on <100> wafers

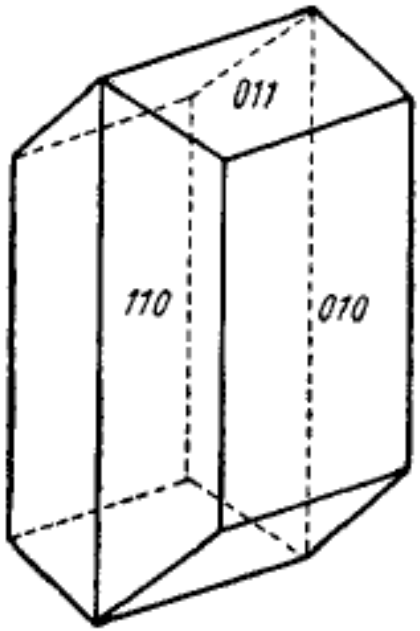


Crystals

rule of rationality

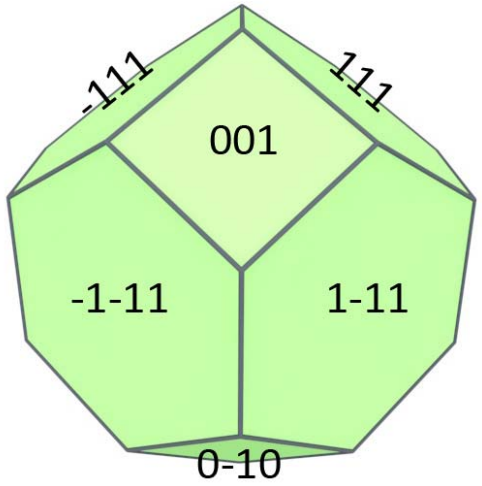
R. J. Haüy (1743-1822):

the indices of external planes of crystals are generally simple full numbers



orthorhombic

Aragonit $CaCO_3$



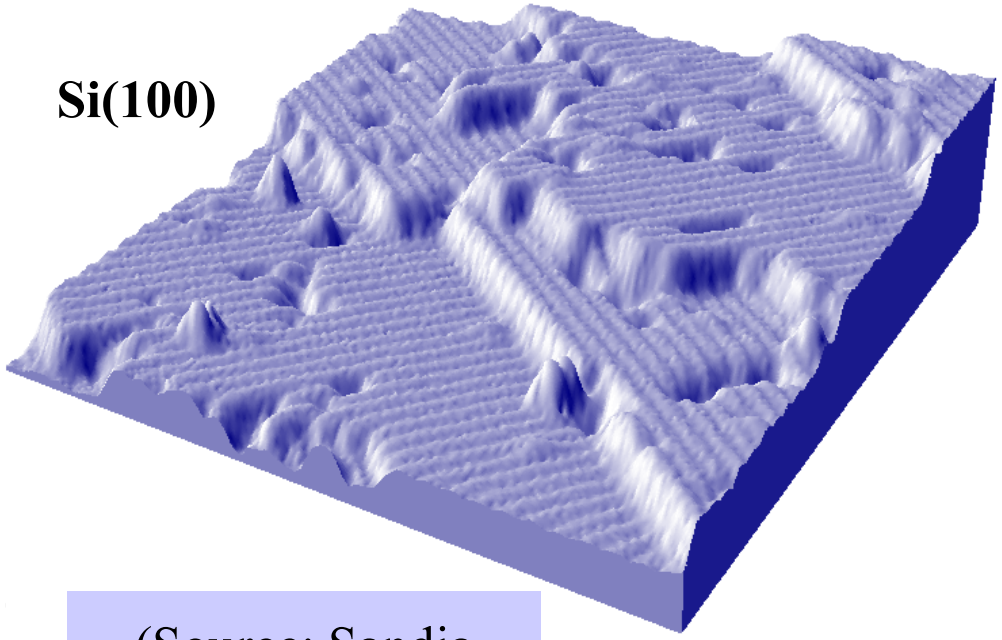
one possible morphology
of a crystal with cubic structure

Bravais:

Planes with high atomic densities tend to dominate

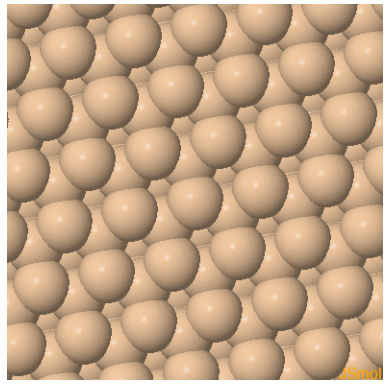
Silicon surfaces

Si(100)

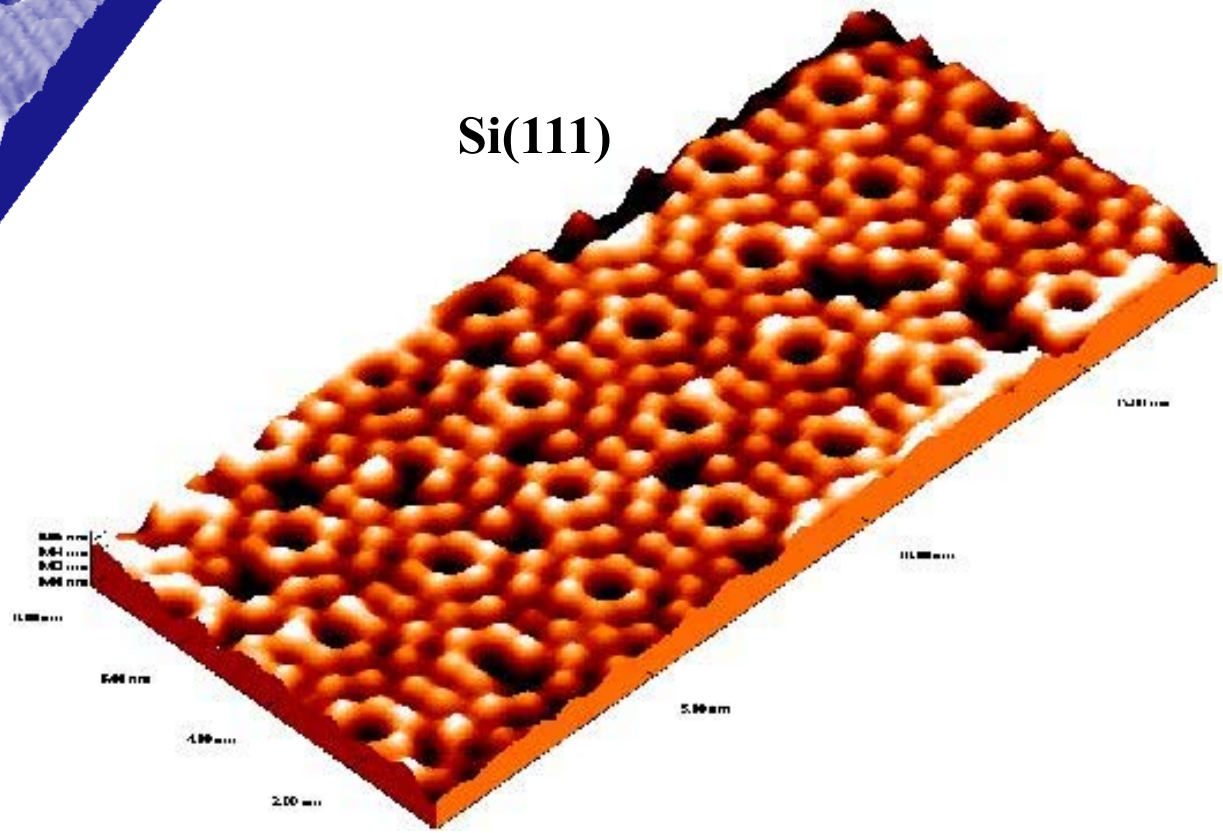


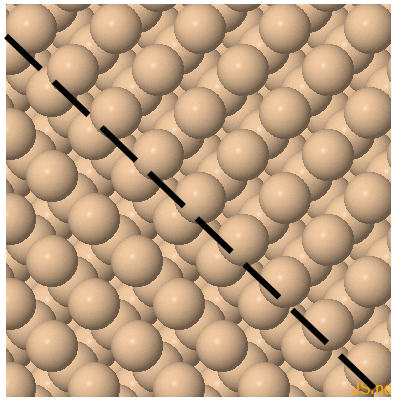
(Source: Sandia Nat.Labs.)

unreconstructed Si(111) →



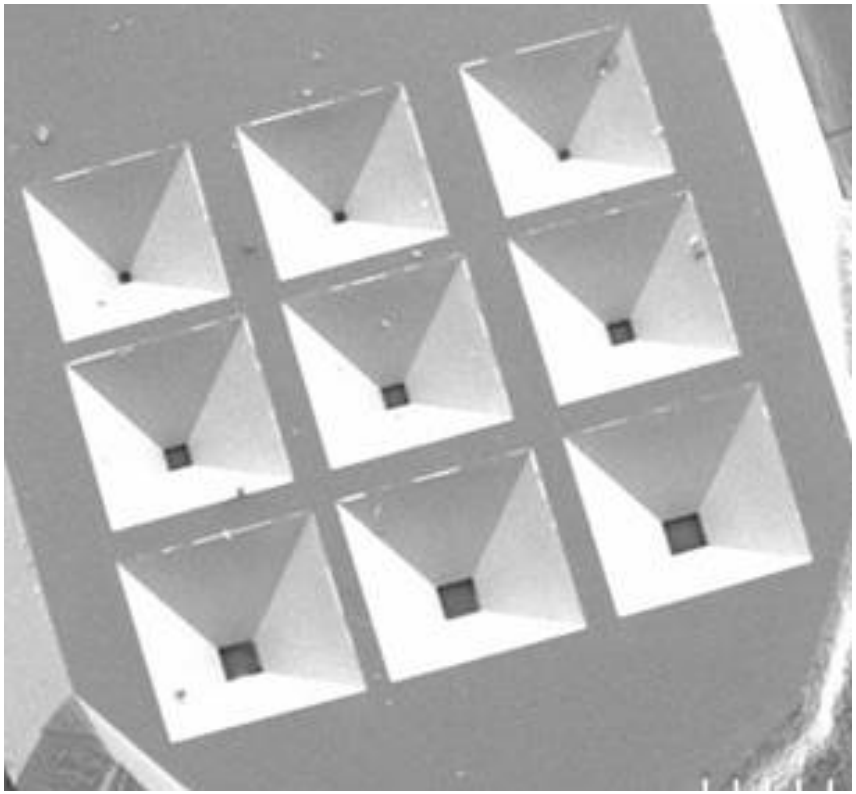
Si(111)





atomic step in Si(100)

KOH etching of silicon

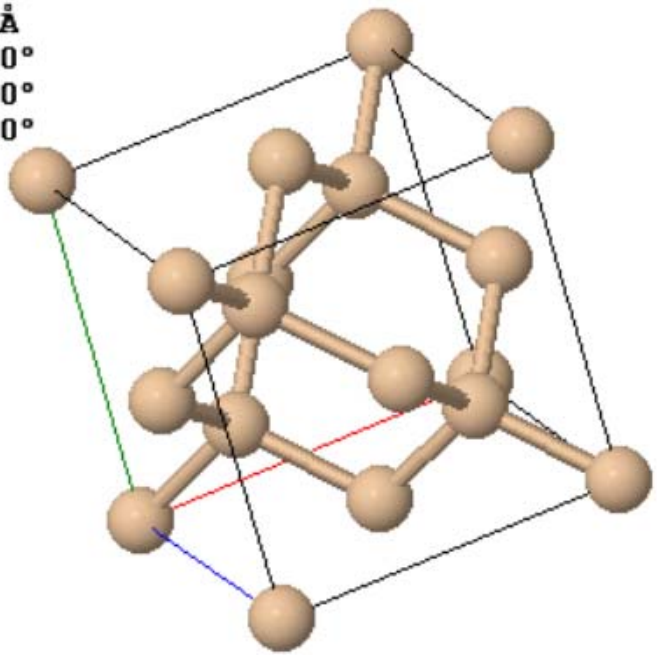


KOH etches Si {110} > {100} > {111}, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

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

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: 1 K: 0 L: 0

show HKL plane | hide HKL plane

draw atoms in HKL plane

Thickness of HKL planes:

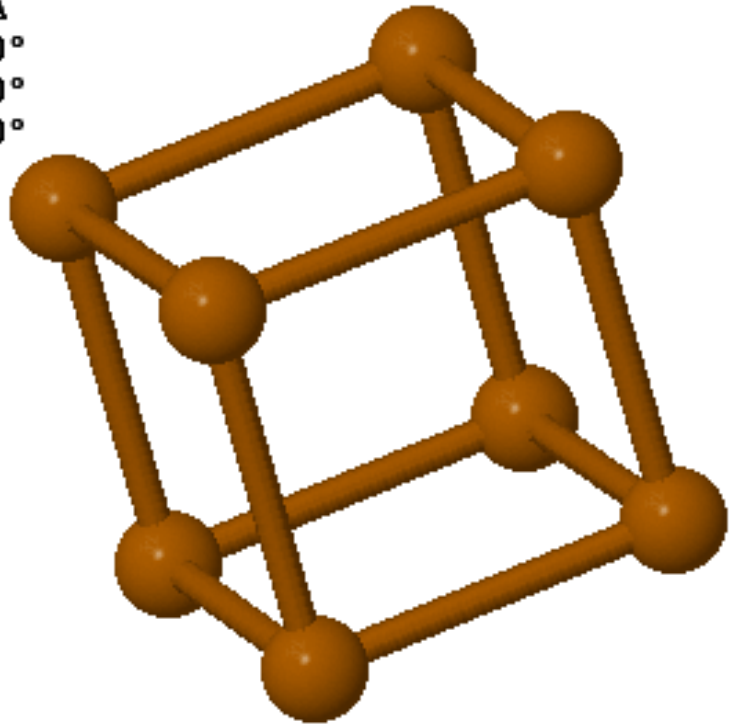
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

simple cubic

Po

HM:P m -3 m
a=3.359Å
b=3.359Å
c=3.359Å
α=90.000°
β=90.000°
γ=90.000°



Number: 221

Primitive Vectors:

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

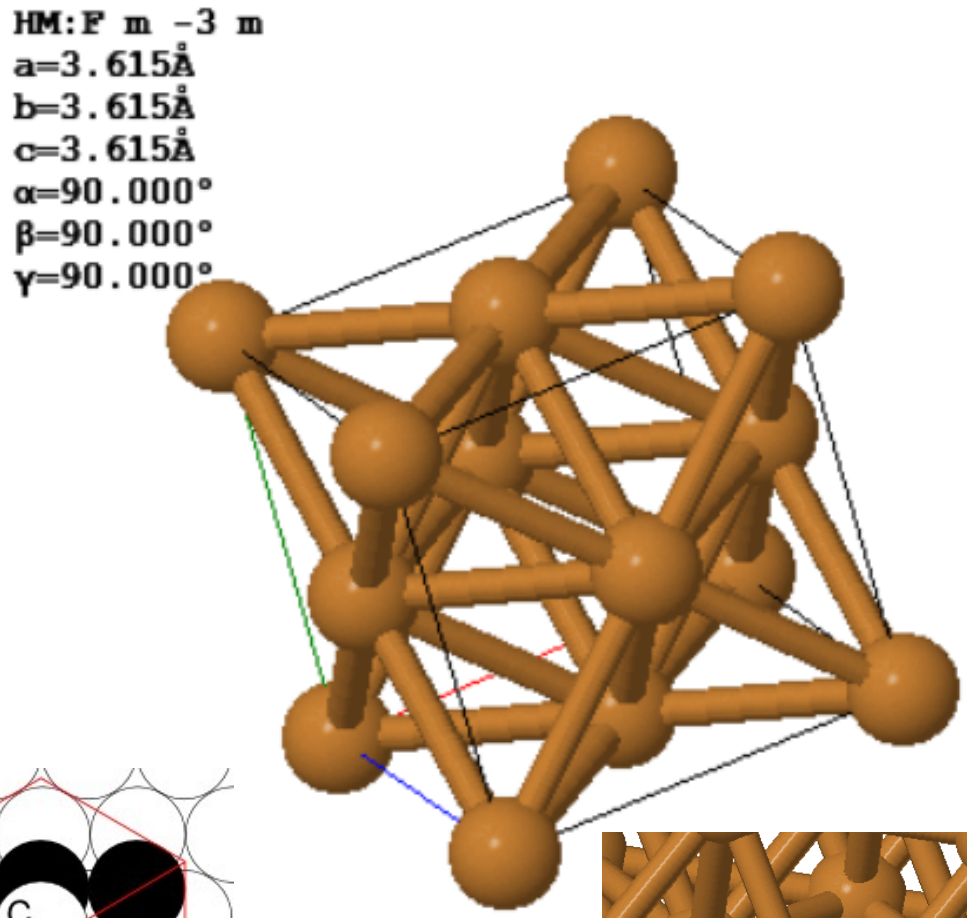
$$\vec{a}_3 = a\hat{z}$$

Basis Vector: $\vec{B}_1 = (0,0,0)$

fcc

Number 225

Al, Cu,
Ni, Sr,
Rh, Pd,
Ag, Ce,
Tb, Ir,
Pt, Au,
Pb, Th



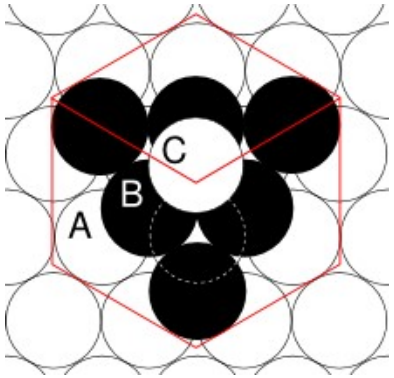
[111]

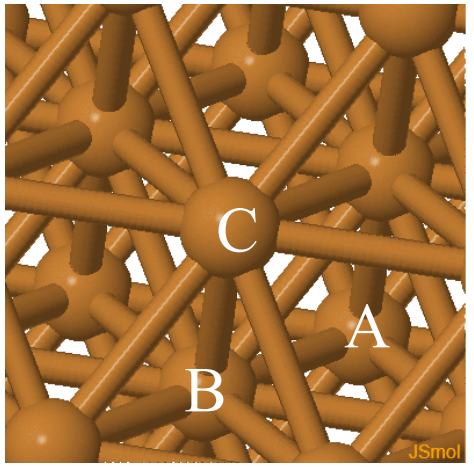
Primitive Vectors:

$$\vec{a}_1 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

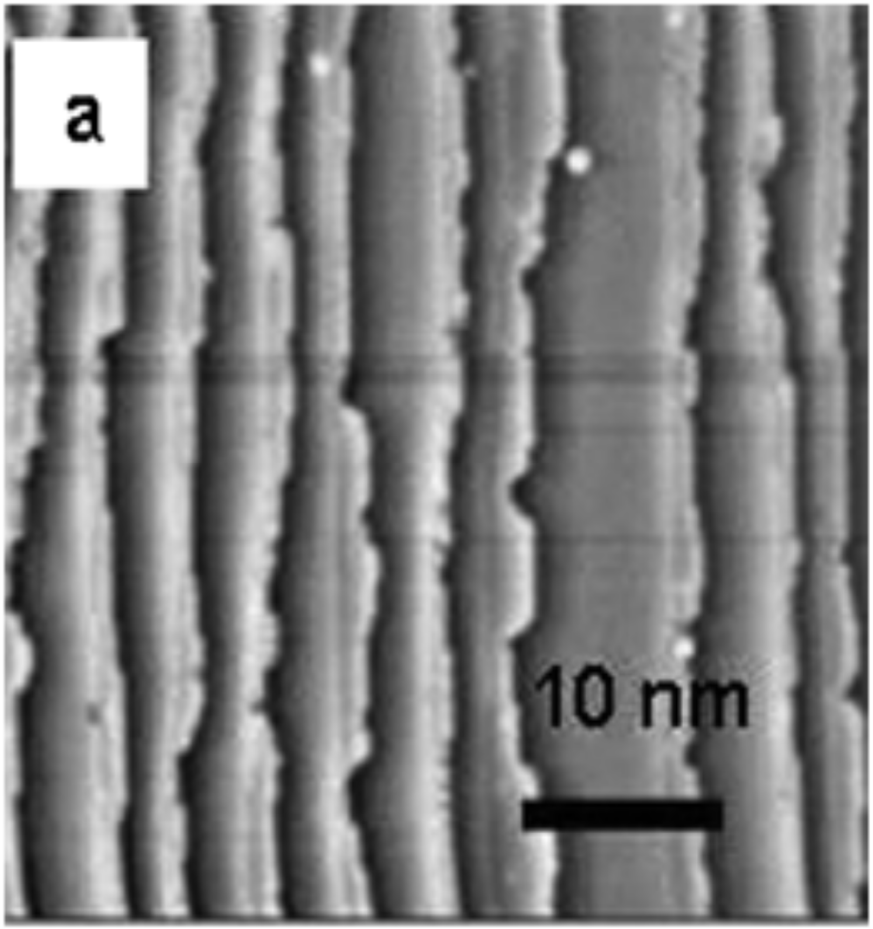
$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$



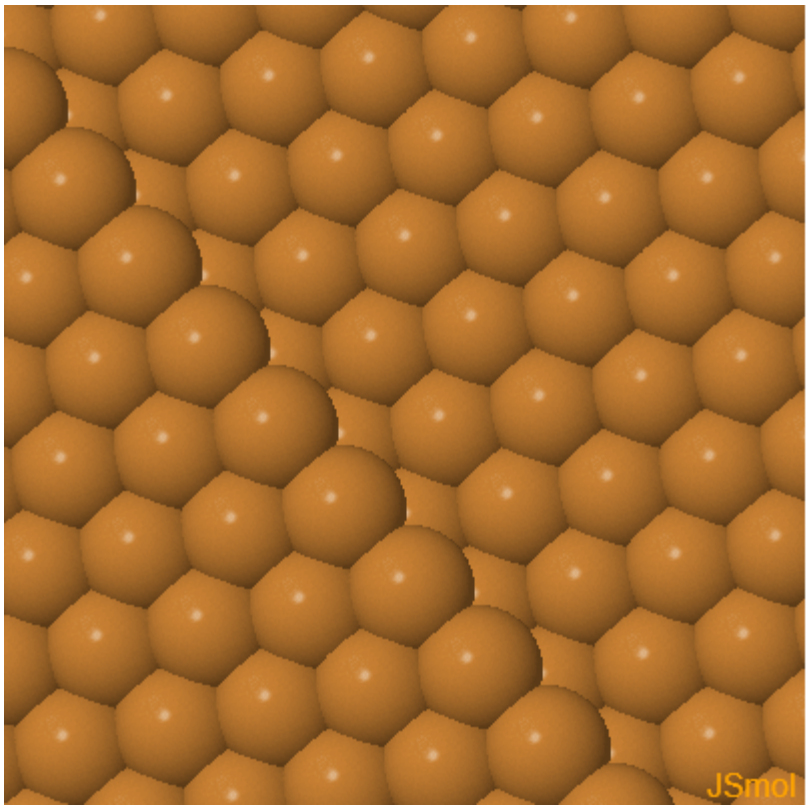


Basis Vector: $\vec{B}_1 = (0,0,0)$

Crystal planes: Miller indices



Rh(15,15,13) fcc



(15,15,13) fcc

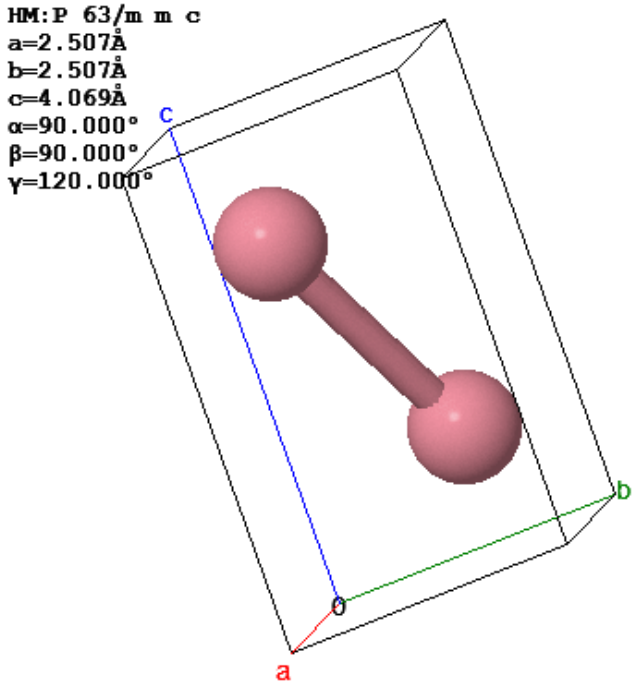
Reaction studies on nanostructured surfaces, Adolf Winkler, in *The Oxford Handbook of Nanoscience and Technology*, A. V. Narlikar and Y. Y. Fu ed., 2009.

hcp

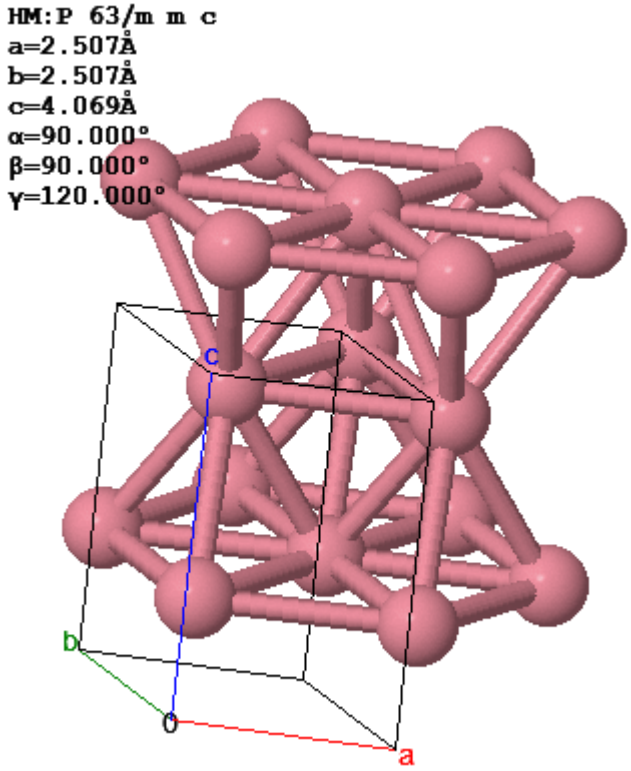
Space group 194

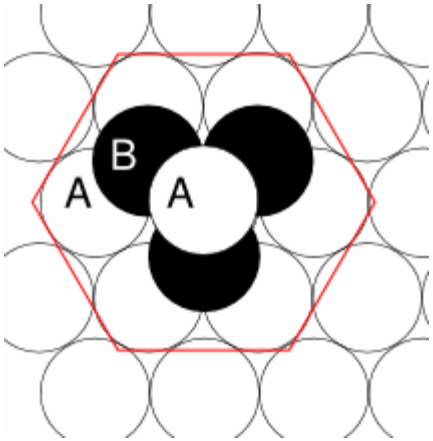
Mg, Be,
Sc, Ti,
Co, Zn,
Y, Zr, Tc,
Ru, Cd,
Gd, Tb,
Dy, Ho,
Er, Tm,
Lu, Hf,
Re, Os,
Tl

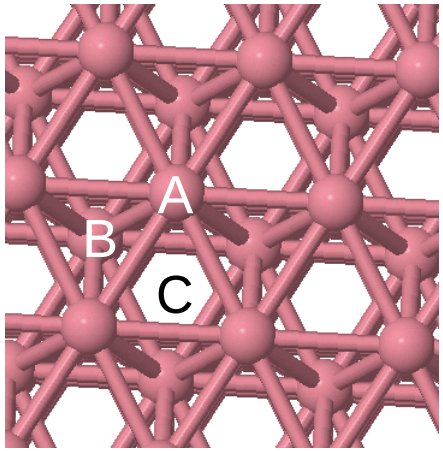
Crystallographic unit cell



Hexagonal unit cell







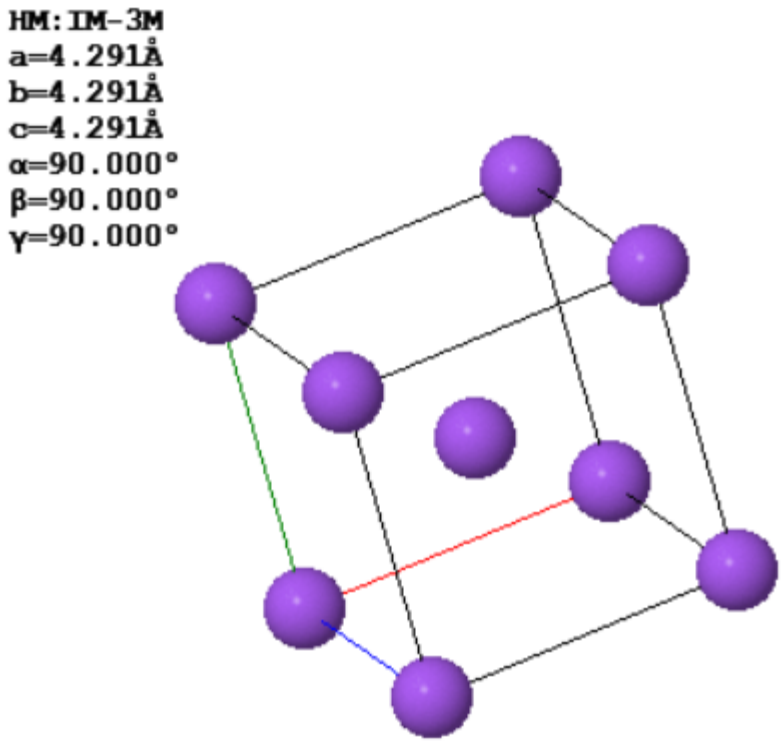
Hexagonal Bravais lattice
Basis vectors:

$$\vec{B}_1 = (0,0,0) \quad \vec{B}_2 = (\tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{2})$$

bcc

W
Na
K
V
Cr
Fe
Rb
Nb
Mo
Cs
Ba
Eu
Ta

Number 229



Primitive Vectors:

$$\vec{a}_1 = -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z}$$

Basis Vector: $\vec{B}_1 = (0,0,0)$

Sodalite

From Wikipedia, the free encyclopedia

Sodalite is a rich royal blue mineral widely enjoyed as an ornamental gemstone. Although massive sodalite samples are opaque, crystals are usually transparent to translucent. Sodalite is a member of the sodalite group with hauyne, nosean, lazurite and tugtupite.

Discovered in 1811 in the Ilimaussaq intrusive complex in Greenland, sodalite did not become important as an ornamental stone until 1891 when vast deposits of fine material were discovered in Ontario, Canada.

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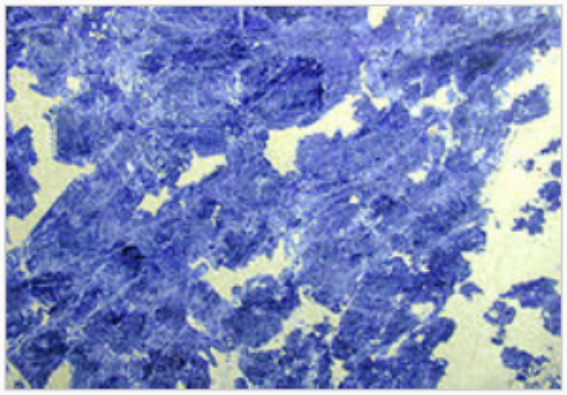
Properties [edit]



A sample of **sodalite**-carbonate pegmatite from Bolivia, with a polished rock

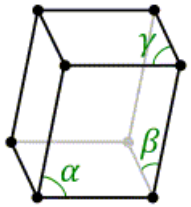
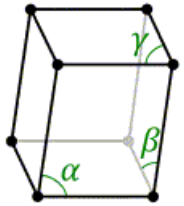
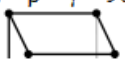
A light, relatively hard yet fragile mineral, sodalite is named after its sodium content; in mineralogy it may be classed as a feldspathoid. Well known for its blue color, sodalite may also be grey, yellow, green, or pink and is often mottled with white veins or patches. The more uniformly blue material is used in jewellery, where it is fashioned into cabochons and beads. Lesser material is more often seen as facing or inlay in

Sodalite

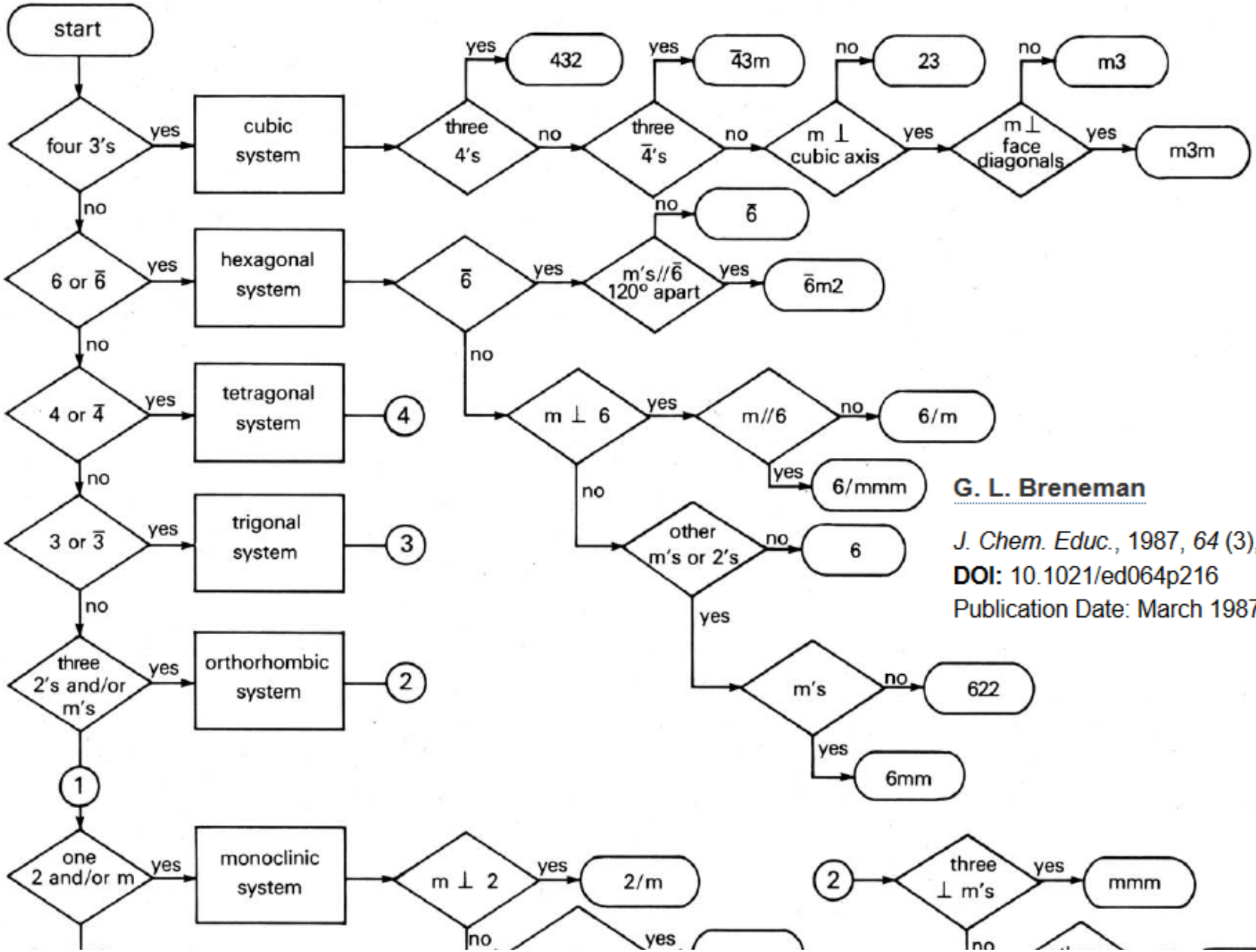
A sample of sodalite

General	
Category	Tectosilicates without zeolitic H_2O
Formula (repeating unit)	$Na_8(Al_6Si_6O_{24})Cl_2$
Strunz classification	09.FB.10
Crystal symmetry	Isometric hextetrahedral H-M symbol: $\bar{4}3m$ Space group: $P\bar{4}3n$
Unit cell	a = 8.876(6) Å; Z = 1
Identification	

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
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: P$\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$, $\beta = \gamma = 90°$ 	monoclinic-sphenoidal	2	C_2	3: P2, 4: P2_1, 5: C2	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6: Pm, 7: Pc, 8: Cm, 9: Cc	-	-	-	-	1	n		2
	monoclinic-prismatic	$2/m$	C_{2h}	10: P2/m, 11: P2_1/m, 12: C2/m, 13: P2/c, 14: P2_1/c, 15: C2/c	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: P222_1, 18: P2_12_12, 19: P$2_12_12_1$, 20: C222_1, 21: C222, 22: F222, 23: I222, 24: I$2_12_12_1$	3	-	-	-	-	n		4

Crystallographic symmetry point group notation flow chart



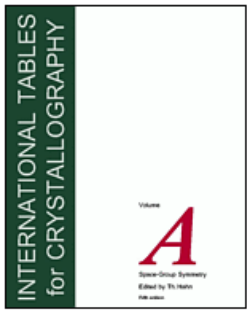
G. L. Breneman

J. Chem. Educ., 1987, *64* (3), p 216
DOI: 10.1021/ed064p216
Publication Date: March 1987

International Tables for Crystallography
Volume A: Space-group symmetry

First online edition (2006) ISBN: 978-0-7923-6590-7 eISBN: 978-1-4020-5406-8 doi: 10.1107/9780955360206000100

Edited by Th. Hahn



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14 (P 21/c)
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18 (P 21 21 2)
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Volume A treats crystallographic symmetry in direct or physical space. It contains extensi rations of the 17 plane groups, the 230 space groups and the 32 crystallographic point groups.

The first five parts of the volume contain introductory material: lists of symbols and terms; e space-group tables; the determination of space groups; synoptic tables of space-grou symbols; and unit-cell (coordinate) transformations. These are followed by the plane-grou les (Parts 6 and 7). For each group type, the following information is presented:

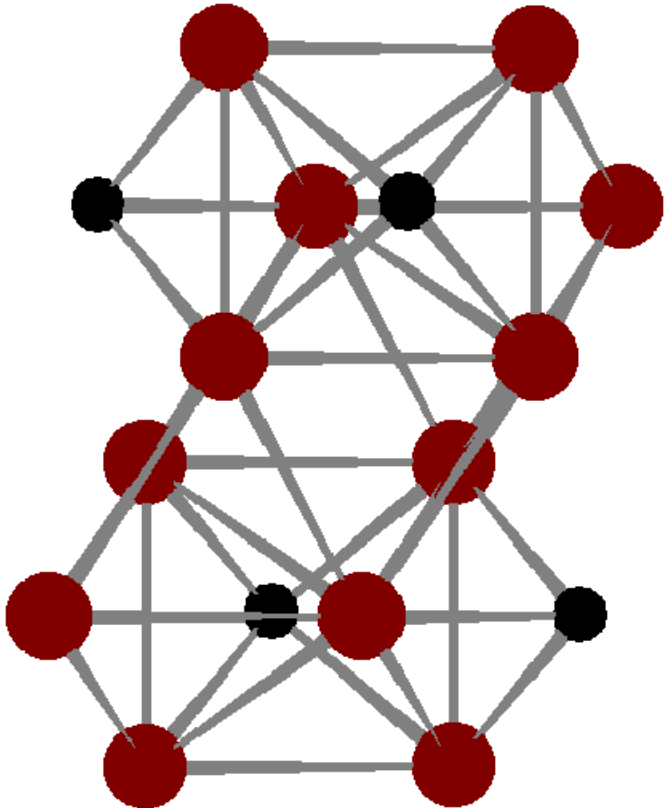
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and re
- symmetries of special projections;
- extensive subgroup and supergroup data.

Parts 8 to 15 deal with the following aspects of symmetry theory: the mathematical approach to space groups; crystal lattices; point groups and crystal classes; symbols for symmetry operations; symbols for space groups; isomorphic subgroups of space groups; lattice complexes; and normalizers of space groups.

Asymmetric unit

cell 5.09000 6.74800 4.52300 90.000 90.000 90.000
natom 3
Fe1 26 0.18600 0.06300 0.32800
Fe2 26 0.03600 0.25000 0.85200
C 6 0.89000 0.25000 0.45000
rgnr 62
Cohenite (Cementite) Fe3 C

Unit cell



Asymmetric unit

Generated by PowderCell