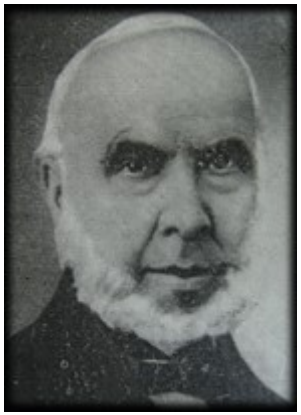
Miller indices

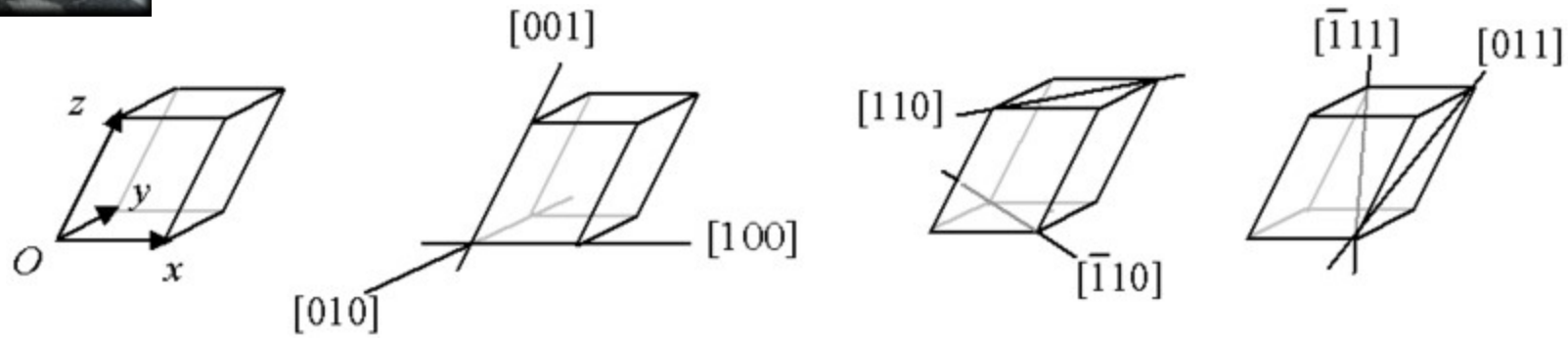
CIF files

Miller indices: Crystal direction [*uvw*]



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

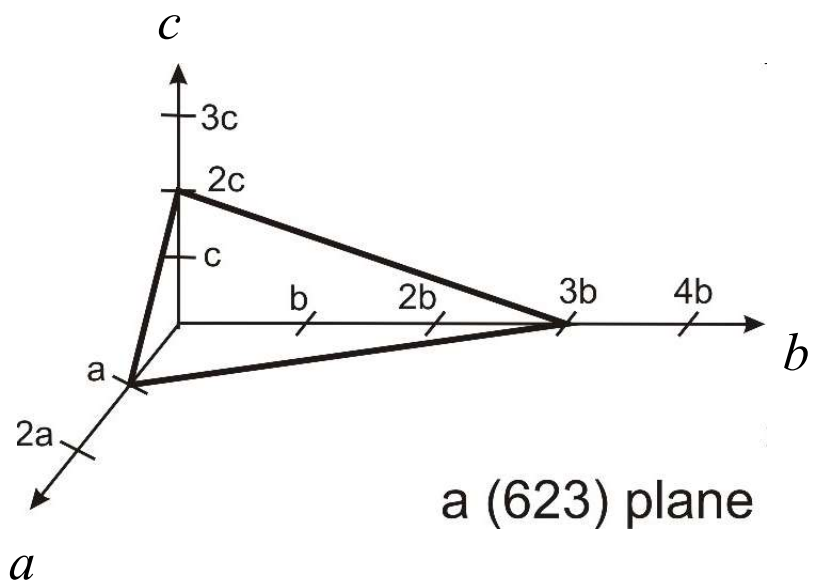
lattice vectors of the crystallographic unit cell



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

[ ] specific direction
< > family of equivalent directions

Miller indices: Crystal planes



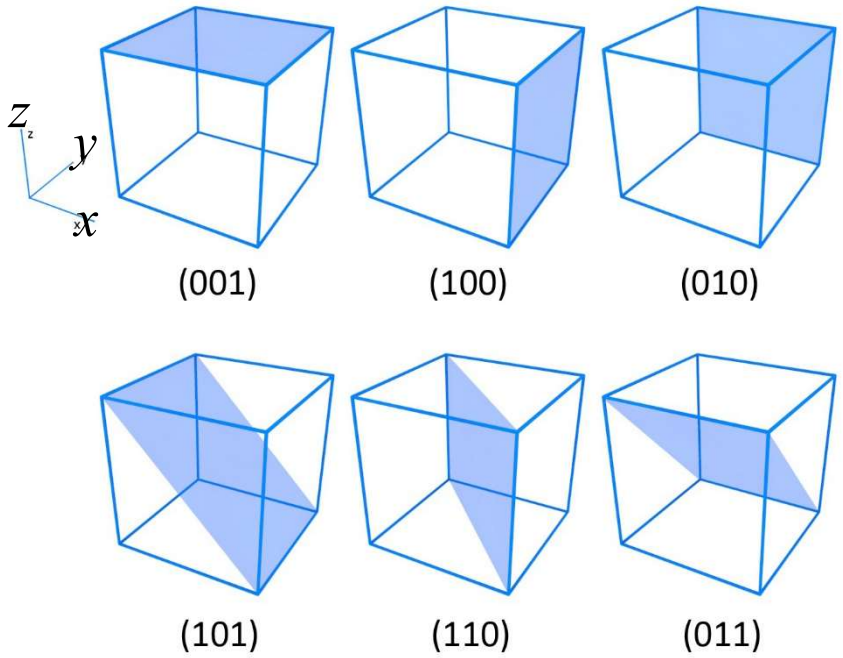
A plane with the intercepts $1/h, 1/k, 1/l$ is the (h,k,l) plane.

always use integers for h,k,l

( ) specific plane

{ } family of equivalent planes

MOSFETs are made on {100} wafers



Miller indices

Primitive lattice vectors:

$\vec{a}_1 =$ 4.12E-10 $\hat{x} +$ 0 $\hat{y} +$ 0 $\hat{z}$ [m]
$\vec{a}_2 =$ 0 $\hat{x} +$ 4.12E-10 $\hat{y} +$ 0 $\hat{z}$ [m]
$\vec{a}_3 =$ 0 $\hat{x} +$ 0 $\hat{y} +$ 4.12E-10 $\hat{z}$ [m]

Miller indices:

$h =$ 1 $k =$ 0 $l =$ 0

submit

Primitive unit cells:

Al (fcc) | W (bcc) | NaCl (fcc) | CsCl (sc) | SrTiO3 (sc) | GaAs (Zincblend, fcc) | GaN (Wurtzite, hex) | YBCO (Orthorhombic)

Conventional unit cells:

Al (fcc) | W (bcc)

The volume of the primitive unit cell is, $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = 6.9935\text{e-}29$ [m³].

The translation vector is, $\vec{T}_{hkl} = 4.12\text{e-}10\ \hat{x} + 0\ \hat{y} + 0\ \hat{z}$ [m].

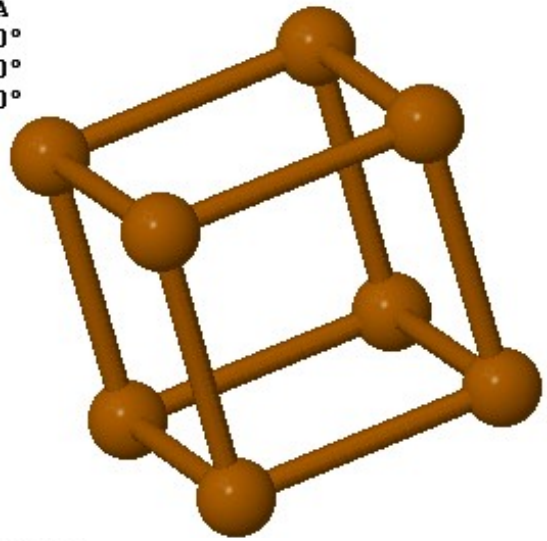
The length of the translation vector is, 4.12e-10 [m].

The normal vector to the (hkl) plane is, $\hat{n}_{hkl} = 1.00\ \hat{x} + 0.00\ \hat{y} + 0.00\ \hat{z}$.

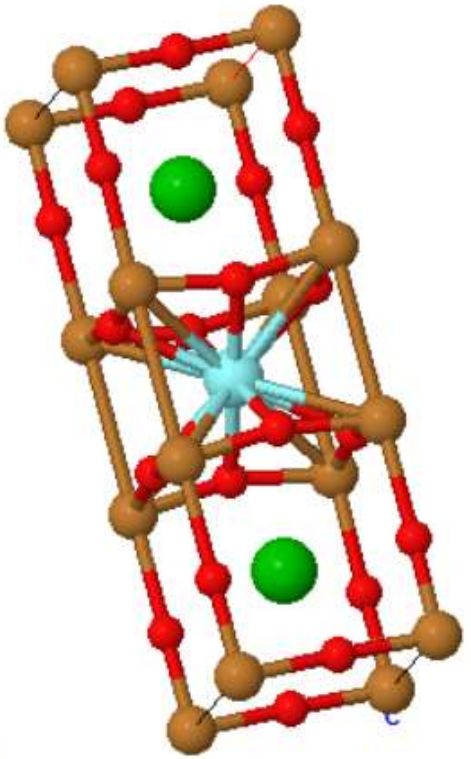
The unit vector in the $\vec{T}_{hkl}$ direction is, $\hat{T}_{hkl} = 1.00\ \hat{x} + 0.00\ \hat{y} + 0.00\ \hat{z}$.

The angle between $\vec{T}_{hkl}$ and $\hat{n}_{hkl}$ is, $\theta = 0.00$ [rad].

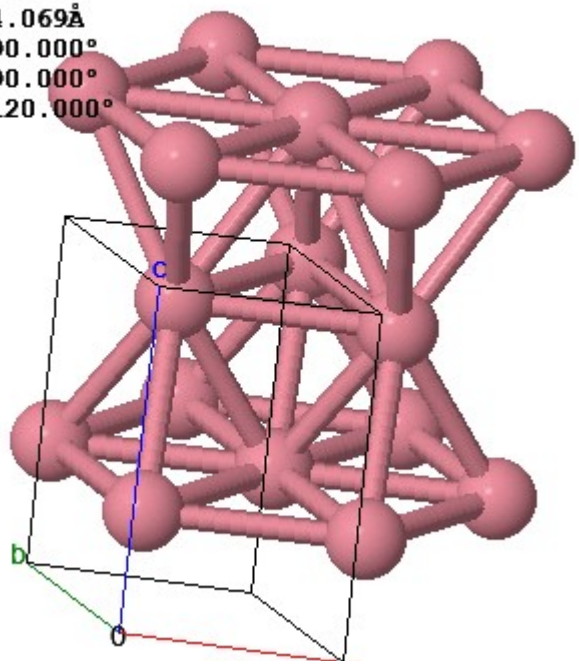
HM:P m -3 m
a=3.359Å
b=3.359Å
c=3.359Å
α=90.000°
β=90.000°
γ=90.000°



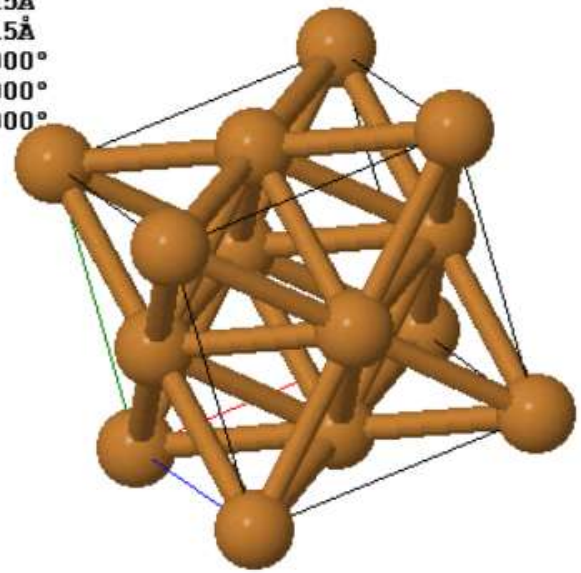
HM:P m m m
a=3.820Å
b=3.885Å
c=11.683Å
α=90.000°
β=90.000°
γ=90.000°



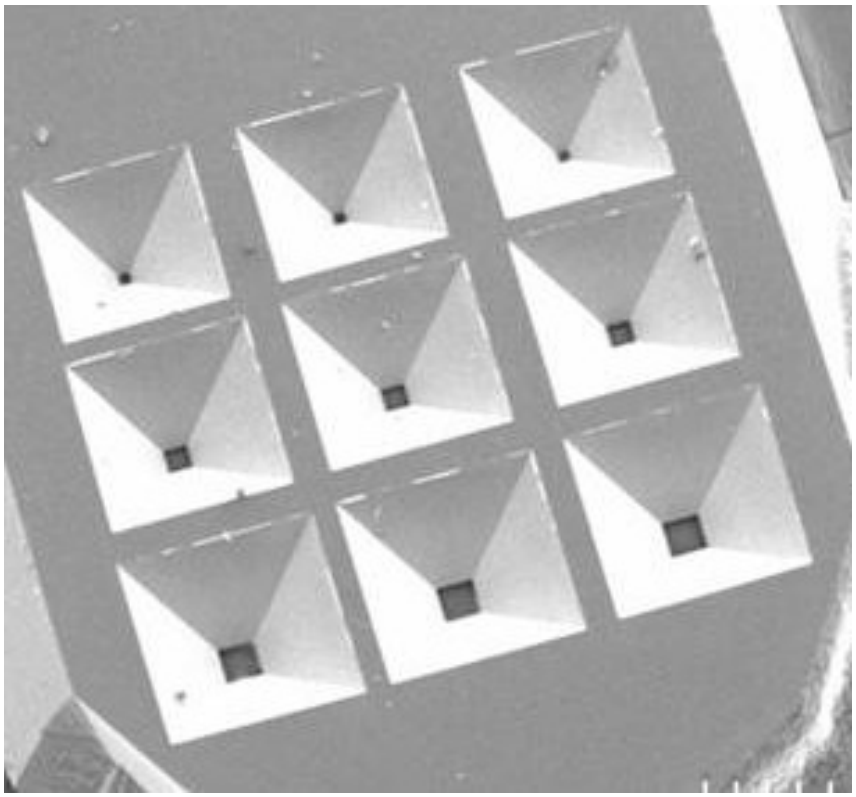
HM:P 63/m m c
a=2.507Å
b=2.507Å
c=4.069Å
α=90.000°
β=90.000°
γ=120.000°



HM:F m -3 m
a=3.615Å
b=3.615Å
c=3.615Å
α=90.000°
β=90.000°
γ=90.000°



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).

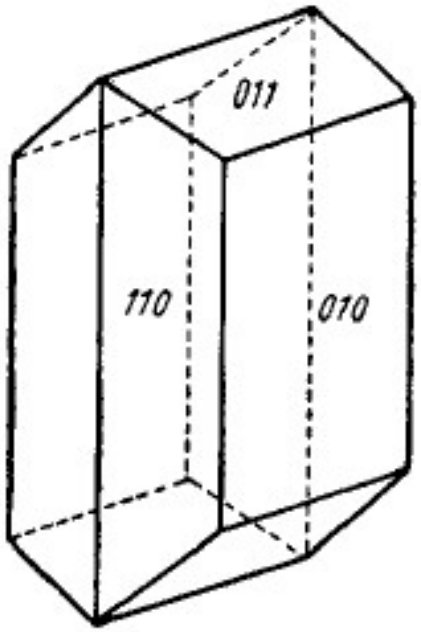
http://www.ece.uncc.edu/research/clean_room/fabprocesses/KOH-EtchingAndDecon.pdf

Crystals

rule of rationality

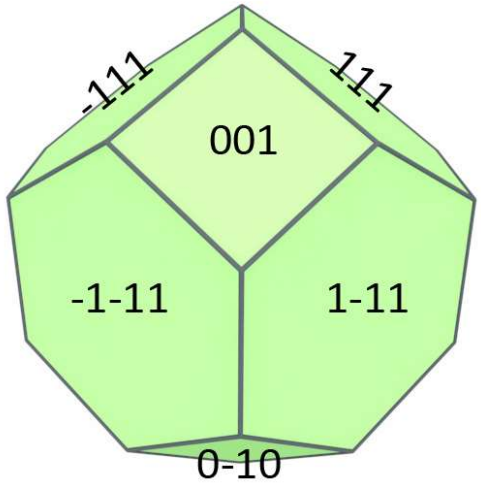
R. J. Haüy (1743-1822):

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



orthorhombic

Aragonit $CaCO_3$



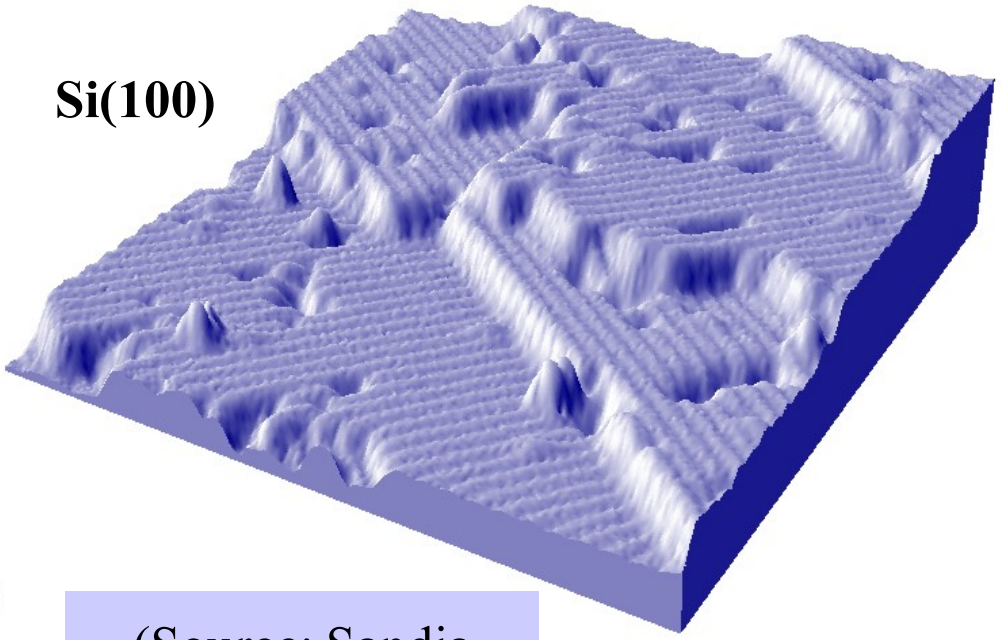
one possible morphology
of a crystal with cubic structure

Bravais:

Planes with high atomic densities tend to dominate

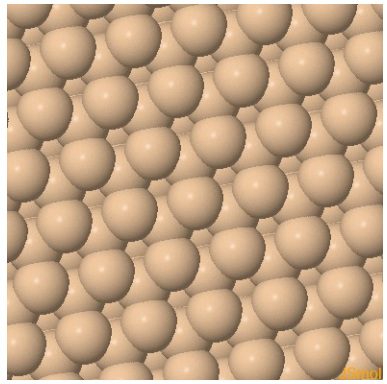
Silicon surfaces

Si(100)

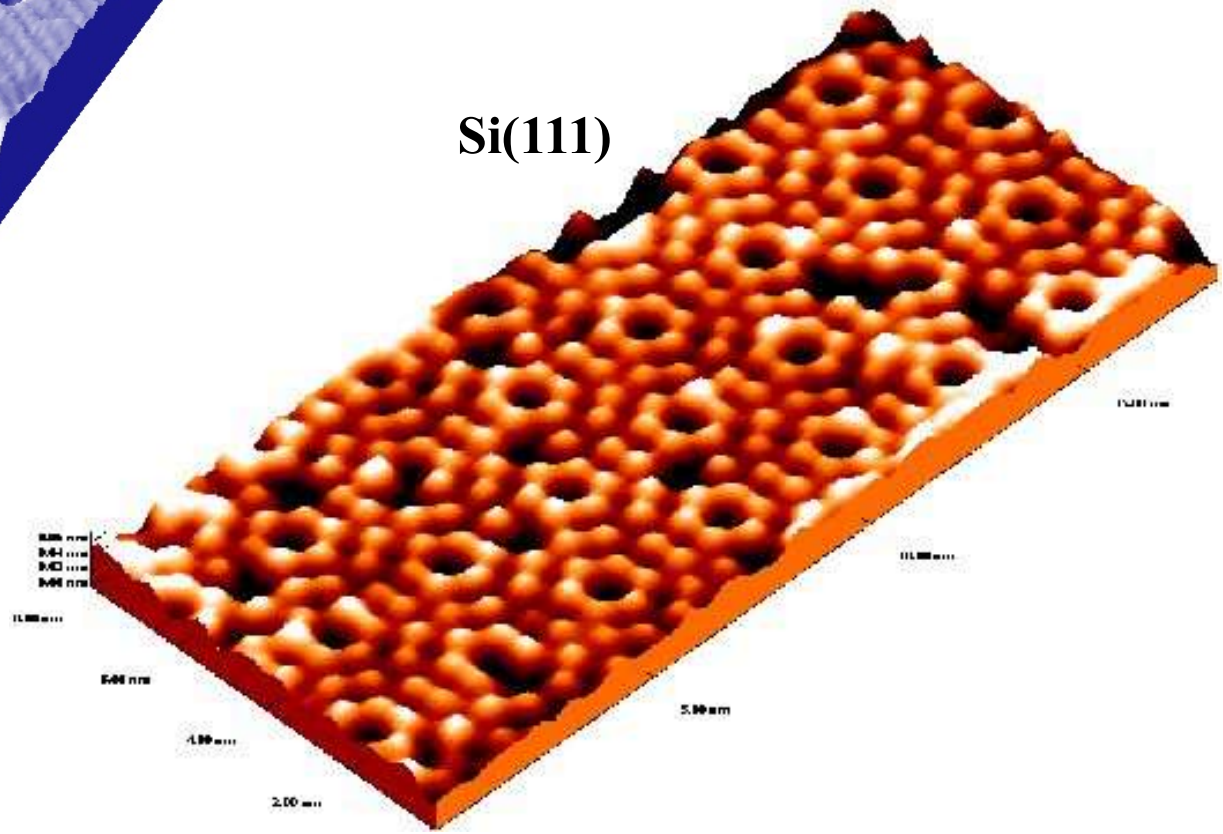


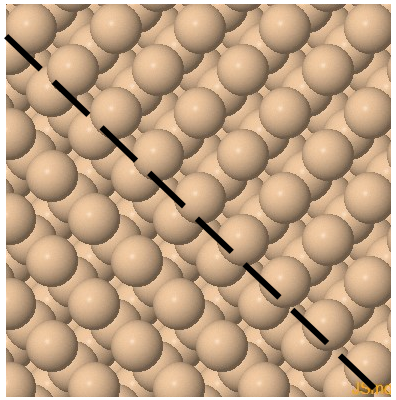
(Source: Sandia Nat.Labs.)

unreconstructed Si(111) →



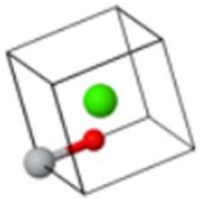
Si(111)



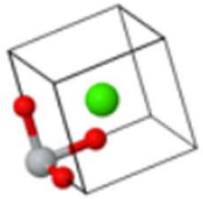


atomic step in Si(100)

Asymmetric unit

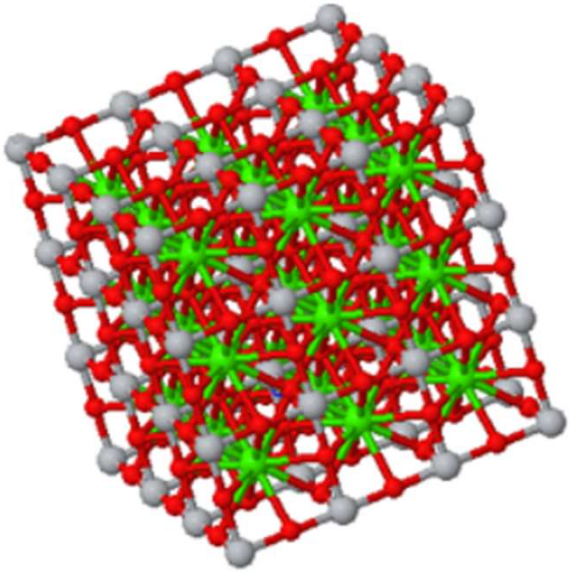


Asymmetric unit



Primitive unit cell

Conventional unit cell

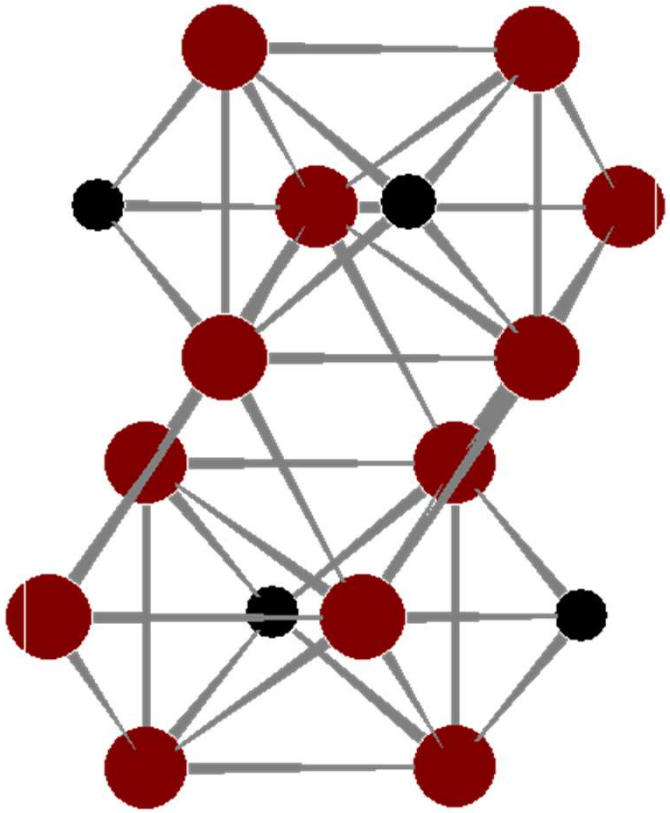


Crystal

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

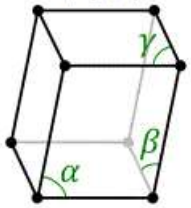
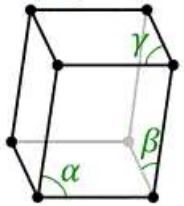
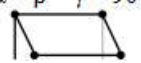
Unit cell



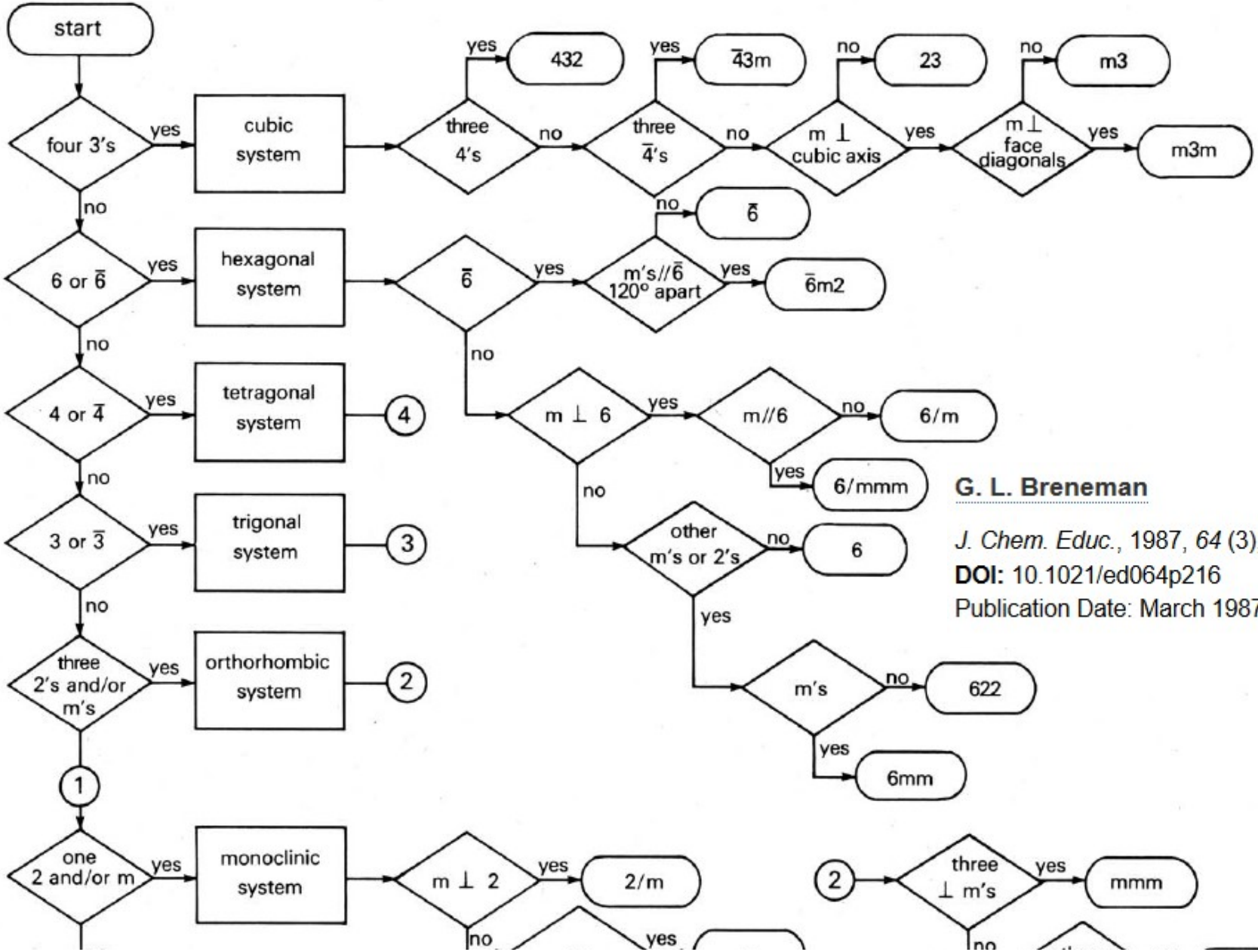
Asymmetric unit

Generated by PowderCell

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$_1$2$_1$2, 19: P2$_1$2$_1$2$_1$, 20: C222$_1$, 21: C222, 22: F222, 23: I222, 24: I2$_1$2$_1$2$_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

http://it.iucr.org/A/

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: 10.1107/97809553602060000100

Edited by Th. Hahn

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| explanation of the space-group data |

Go to space group No. 1 (P 1) Go

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2 (P -1)
3 (P 2)
4 (P 21)
5 (C 2)
6 (P m)
7 (P c)
8 (C m)
9 (C c)
10 (P 2/m)
11 (P 21/m)
12 (C 2/m)
13 (P 2/c)
14 (P 21/c)
15 (C 2/c)
16 (P 2 2 2)
17 (P 2 2 21)
18 (P 21 21 2)
19 (P 21 21 21)
20 (C 2 2 21)

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.

CIF files and programs to visualize crystal structures

Crystal structure data is often stored in a CIF file. This is a text file that contains the asymmetric unit of the crystal, the symmetries of the space group, and a reference to the source where the data was first published. It is important to check the publication to see the conditions used during the experiment. Some experiments are performed at high temperatures or high pressures where the crystal structure can be different than at room temperature and ambient pressure. The links below will display a crystal structure and it's corresponding CIF file.

Simple Cubic, Polonium Po $Pm\bar{3}m$ #221
Face-centered Cubic (fcc) $Fm\bar{3}m$ #225
Body-centered Cubic (bcc) $Im\bar{3}m$ #229
Hexagonal, Boron nitride BN #194
Hexagonal Close Packed (hcp) P63/mmc #194
Perovskite, Calcium titanate $CaTiO_3$ (perovskite) $Pm\bar{3}m$ #221
Caesium chloride CsCl $Pm\bar{3}m$ #221
Rocksalt NaCl $Fm\bar{3}m$ #225
Zincblende #216
Wurtzite #186
Diamond (C) #227
β-Sn #141
Graphite C P63mc #186

Sucrose P21 #4
Magnetite Fe_3O_4 Fd3m #227
Cementite Fe_3C #62
Copper oxide CO (Tenorite) #15
Pyrite FeS_2 #205
Rutile TiO_2 #136
Spinel $MgAl_2O_4$ #227
$Sr_2FeMoO6_6$ (double perovskite) I4/mmm #139
$YBa_2Cu_3O_7$ #47
ZIF8 #1
Zinc oxide ZnO (wurtzite) P63mc #186
ZnS (wurtzite) #186

Prototypes | Periodic Table | Semiconductors | Ceramics

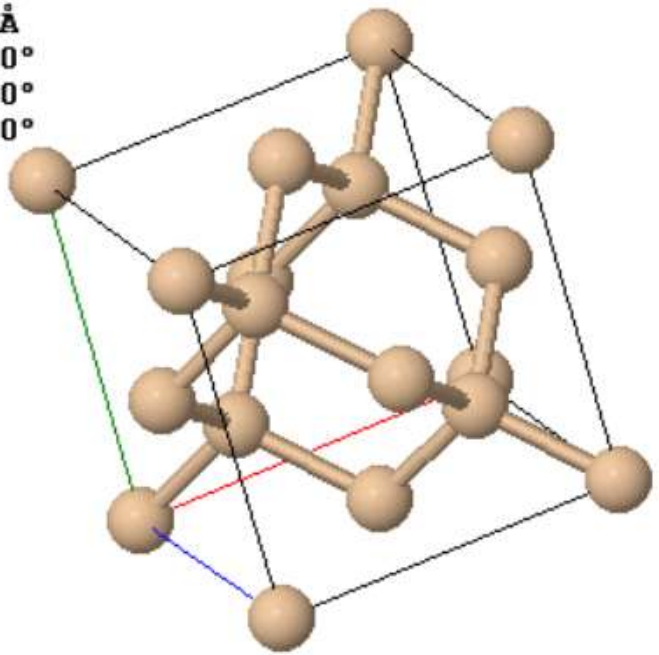
ICSD

Inorganic Crystal Structure Database

Materials Project

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

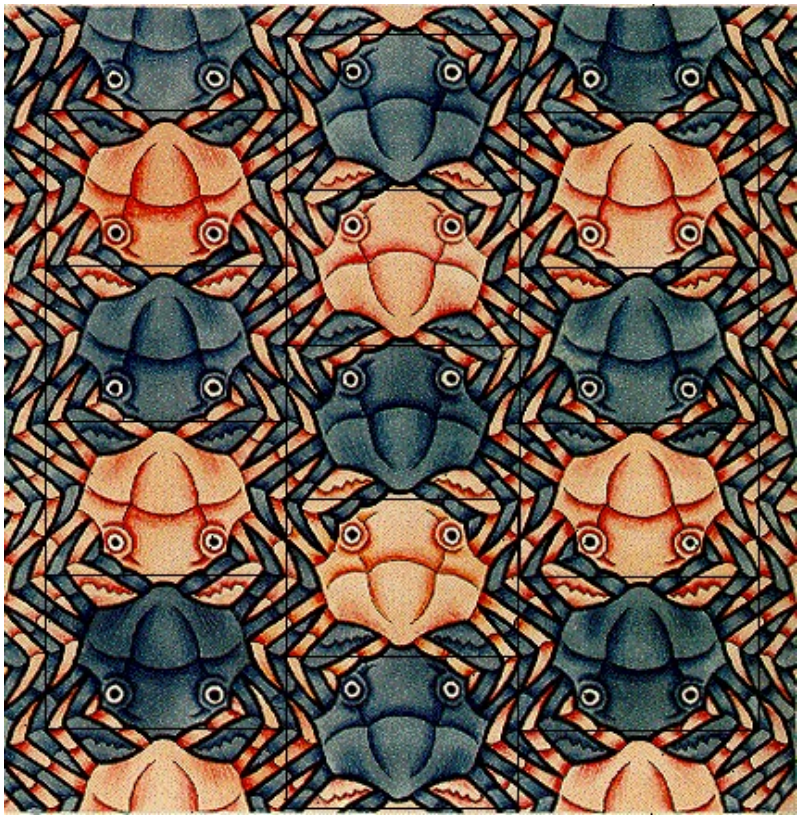
draw atoms in HKL plane

Thickness of HKL planes:

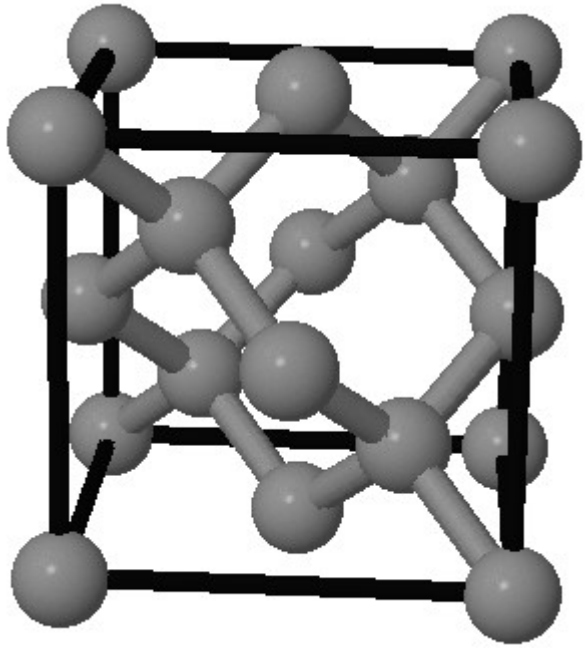
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

Inequivalent atoms in the unit cell



An element can have two distinct positions



Diamond conventional unit cell