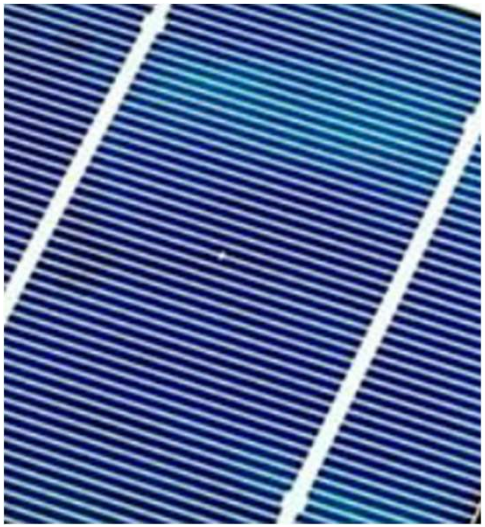
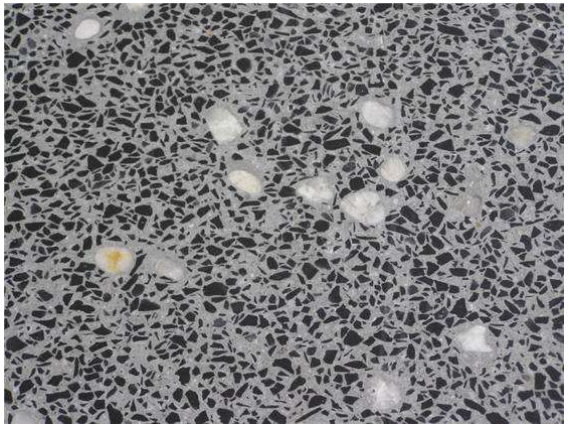
# Introduction to Solid State Physics

Peter Hadley

# Solid materials

Metals and alloys
Plastics
Ceramics
Biological materials
Composite materials

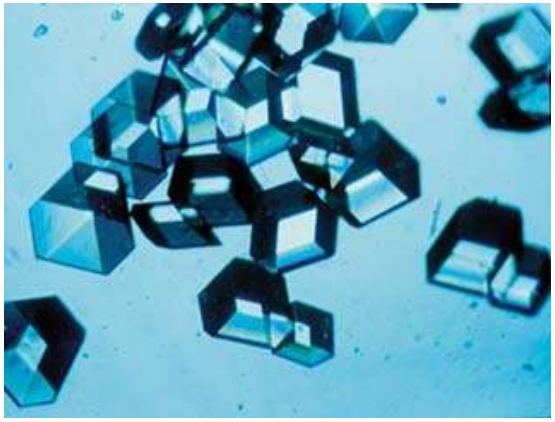




# Crystal = periodic arrangement of atoms

quartz

Gallium crystals



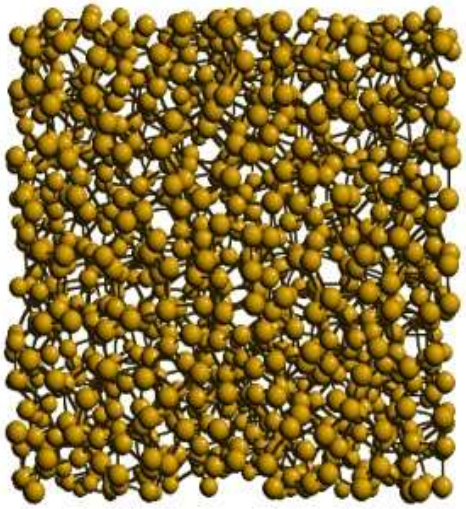
Insulin crystals

http://www.pmc.umontreal.ca/~mousseau/site_an/uploads/Main/si1000.jpg

http://www.wikipedia.org

glass

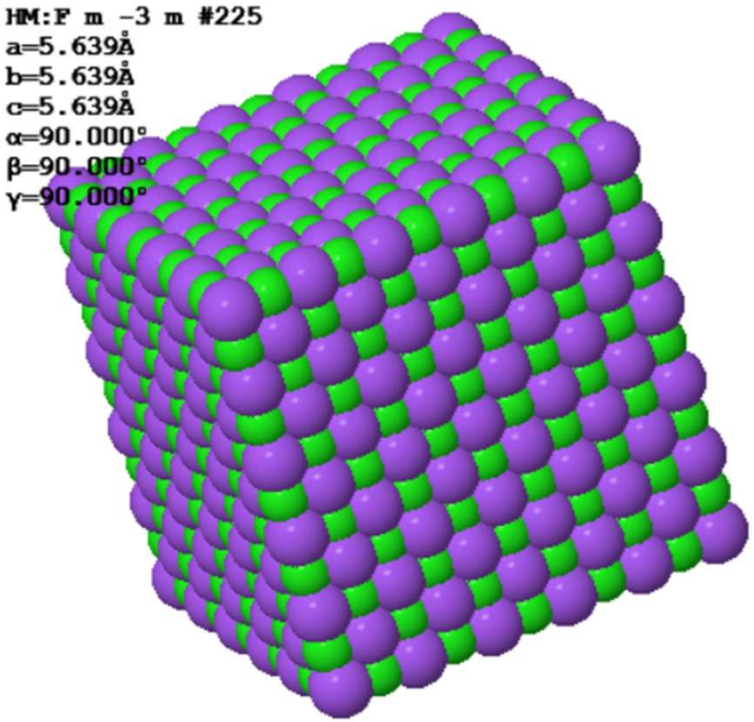
amorphous metal



amorphous silicon

# Goal

From the microscopic structure calculate any property of any solid.




Cooking → Calculating

http://lampx.tugraz.at/~hadley/mas

TU Graz

Print version

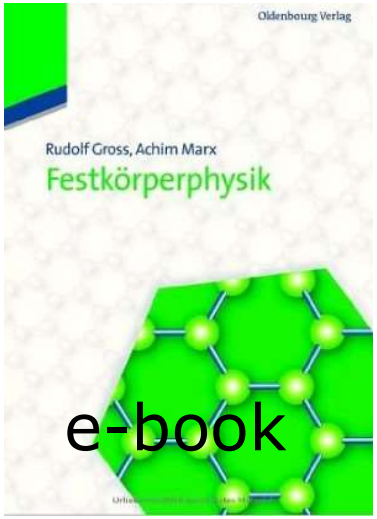
**MAS.020UF Introduction to Solid State Physics**

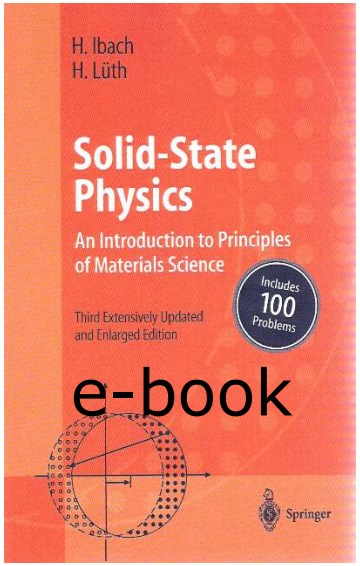


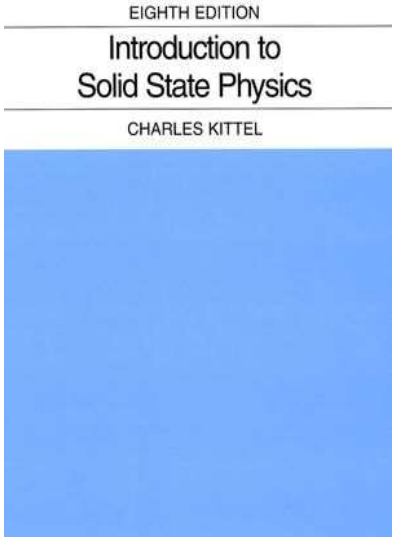
# Course outline

- **Crystal structure**
  - Crystal structure W
  - Unit cell W
  - Bravais lattices W
  - Miller indices W
  - Wigner Seitz cell W
    - Drawing Wigner-Seitz cells
  - Asymmetric unit
  - Examples of crystal structures
    - simple cubic, fcc, bcc, hcp, diamond, silicon, zincblende, ZnO wurzite, NaCl, CsCl, perovskite, graphite, sugar
    - More crystal structures, CIF files, and programs to visualize crystal structures
  - Symmetries
    - Point groups W
      - Table of crystal classes and their associated point groups
      - Flowchart to determine the point group of a crystal
    - Space groups W
    - Space group → Bravais lattice
- **Crystal physics**
  - SGTE data for pure elements - The Gibbs energy as a function of temperature for many

# Books




ICSD

Inorganic Crystal Structure Database

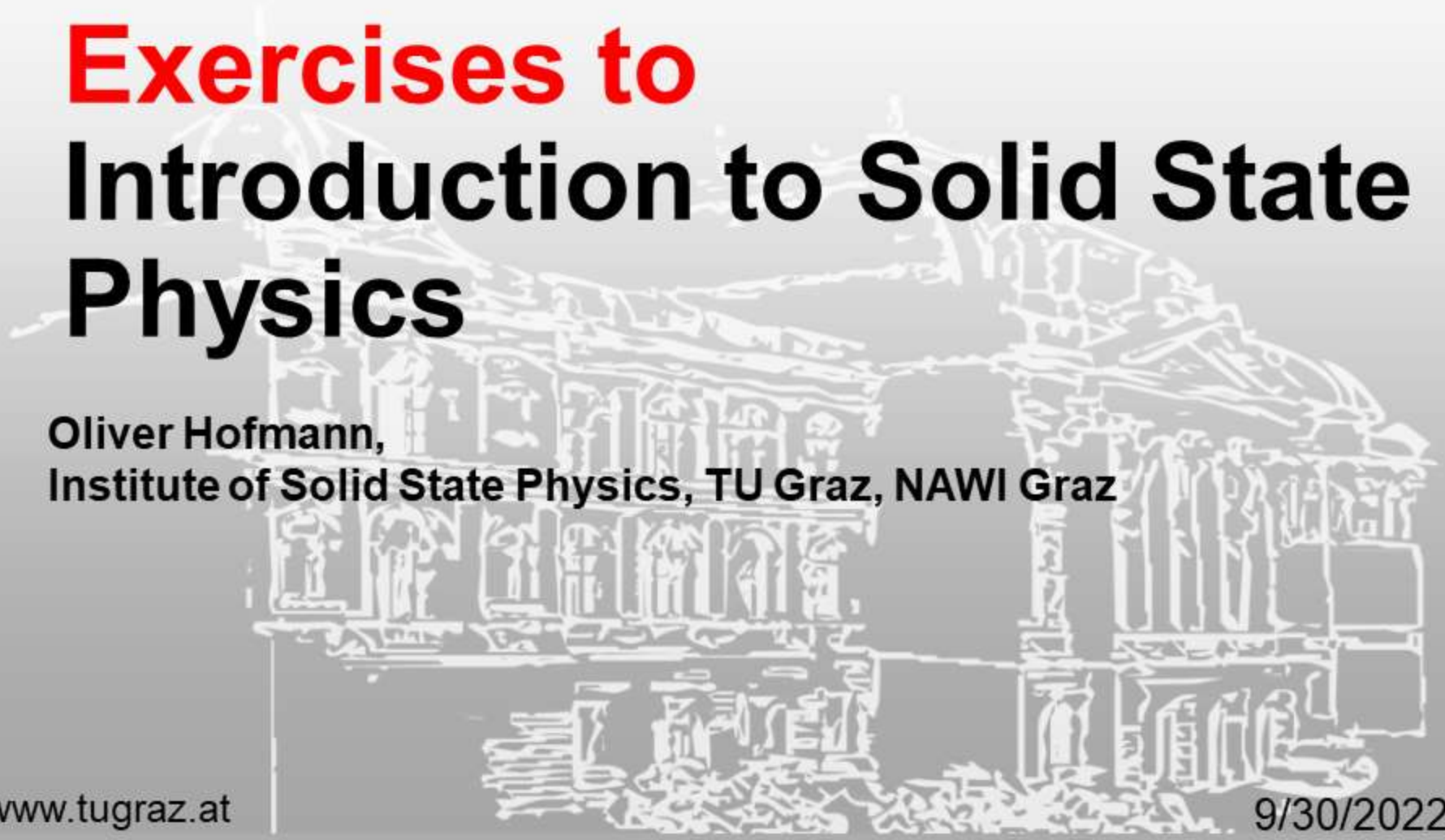
Materials Project

SCIENCE • PASSION • TECHNOLOGY

TU Graz

# Exercises to Introduction to Solid State Physics

**Oliver Hofmann,**
**Institute of Solid State Physics, TU Graz, NAWI Graz**



# Purpose

- Repetition
- Examples and Training
- Identifying open questions
- Preparation for the Exam
- (Potential exam question will be given)

# Procedure

**Place:** to be decided

**Languange:** as requested (German / English)

**Implementation** 7 x 90 min :

***Mandatory Presence!***

# Exam

Written exam on November 23.
Similar to other written exams.

# Carbon polytypes

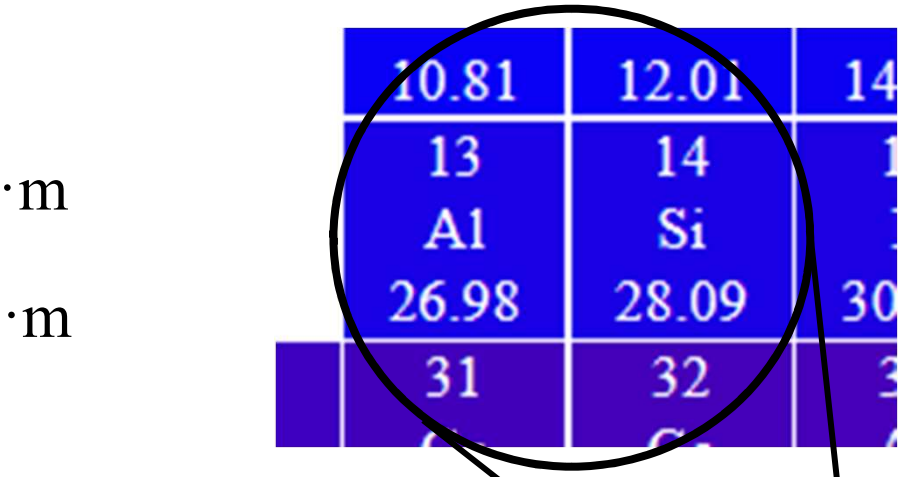
Different polytypes ⇨ Different properties

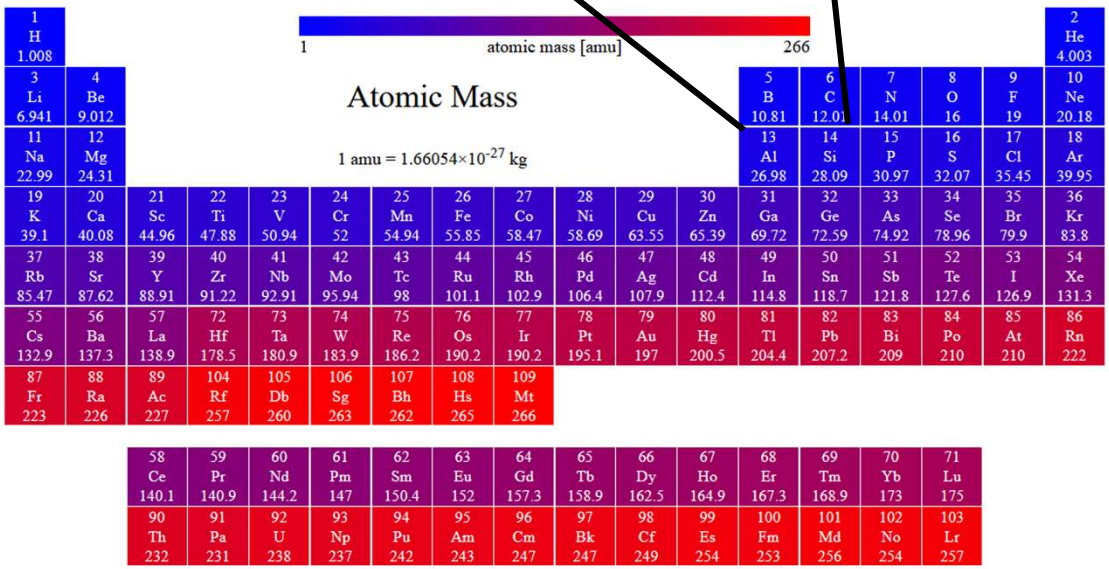
# Aluminum and Silicon

Conductivity

Al: $\sigma = 3.5 \times 10^{7}\ 1/\Omega \cdot m$

Si: $\sigma = 4.3 \times 10^{-4}\ 1/\Omega \cdot m$



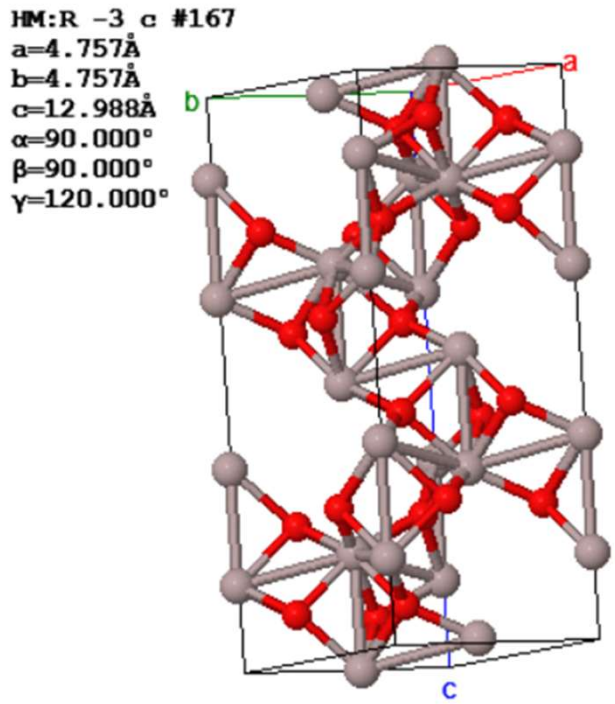




| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 H 1.008 | | | | | | | | | | | | | | | | | 2 He 4.003 |
| 3 Li 6.941 | 4 Be 9.012 | | | | | | | | | | | 5 B 10.81 | 6 C 12.01 | 7 N 14.01 | 8 O 16 | 9 F 19 | 10 Ne 20.18 |
| 11 Na 22.99 | 12 Mg 24.31 | | | | | | | | | | | 13 Al 26.98 | 14 Si 28.09 | 15 P 30.97 | 16 S 32.07 | 17 Cl 35.45 | 18 Ar 39.95 |
| 19 K 39.1 | 20 Ca 40.08 | 21 Sc 44.96 | 22 Ti 47.88 | 23 V 50.94 | 24 Cr 52 | 25 Mn 54.94 | 26 Fe 55.85 | 27 Co 58.47 | 28 Ni 58.69 | 29 Cu 63.55 | 30 Zn 65.39 | 31 Ga 69.72 | 32 Ge 72.59 | 33 As 74.92 | 34 Se 78.96 | 35 Br 79.9 | 36 Kr 83.8 |
| 37 Rb 85.47 | 38 Sr 87.62 | 39 Y 88.91 | 40 Zr 91.22 | 41 Nb 92.91 | 42 Mo 95.94 | 43 Tc 98 | 44 Ru 101.1 | 45 Rh 102.9 | 46 Pd 106.4 | 47 Ag 107.9 | 48 Cd 112.4 | 49 In 114.8 | 50 Sn 118.7 | 51 Sb 121.8 | 52 Te 127.6 | 53 I 126.9 | 54 Xe 131.3 |
| 55 Cs 132.9 | 56 Ba 137.3 | 57 La 138.9 | 72 Hf 178.5 | 73 Ta 180.9 | 74 W 183.9 | 75 Re 186.2 | 76 Os 190.2 | 77 Ir 190.2 | 78 Pt 195.1 | 79 Au 197 | 80 Hg 200.5 | 81 Tl 204.4 | 82 Pb 207.2 | 83 Bi 209 | 84 Po 210 | 85 At 210 | 86 Rn 222 |
| 87 Fr 223 | 88 Ra 226 | 89 Ac 227 | 104 Rf 257 | 105 Db 260 | 106 Sg 263 | 107 Bh 262 | 108 Hs 265 | 109 Mt 266 | | | | | | | | | |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 58 Ce 140.1 | 59 Pr 140.9 | 60 Nd 144.2 | 61 Pm 147 | 62 Sm 150.4 | 63 Eu 152 | 64 Gd 157.3 | 65 Tb 158.9 | 66 Dy 162.5 | 67 Ho 164.9 | 68 Er 167.3 | 69 Tm 168.9 | 70 Yb 173 | 71 Lu 175 |
| 90 Th 232 | 91 Pa 231 | 92 U 238 | 93 Np 237 | 94 Pu 242 | 95 Am 243 | 96 Cm 247 | 97 Bk 247 | 98 Cf 249 | 99 Es 254 | 100 Fm 253 | 101 Md 256 | 102 No 254 | 103 Lr 257 |

# Sapphire and Ruby

Ti




$Al_2O_3$

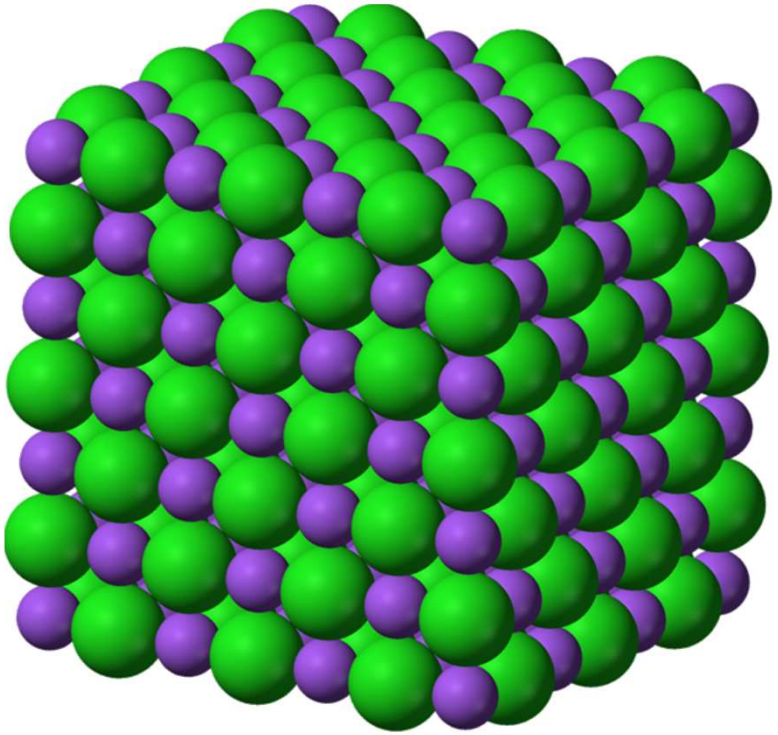
Cr

https://en.wikipedia.org/wiki/Ruby#/media/File:Ruby_gem.JPG
https://en.wikipedia.org/wiki/Sapphire#/media/File:Geschliffener_blauer_Saphir.jpg

# Crystal structure

# 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 $\alpha \neq 90° \ \beta = \gamma = 90°$

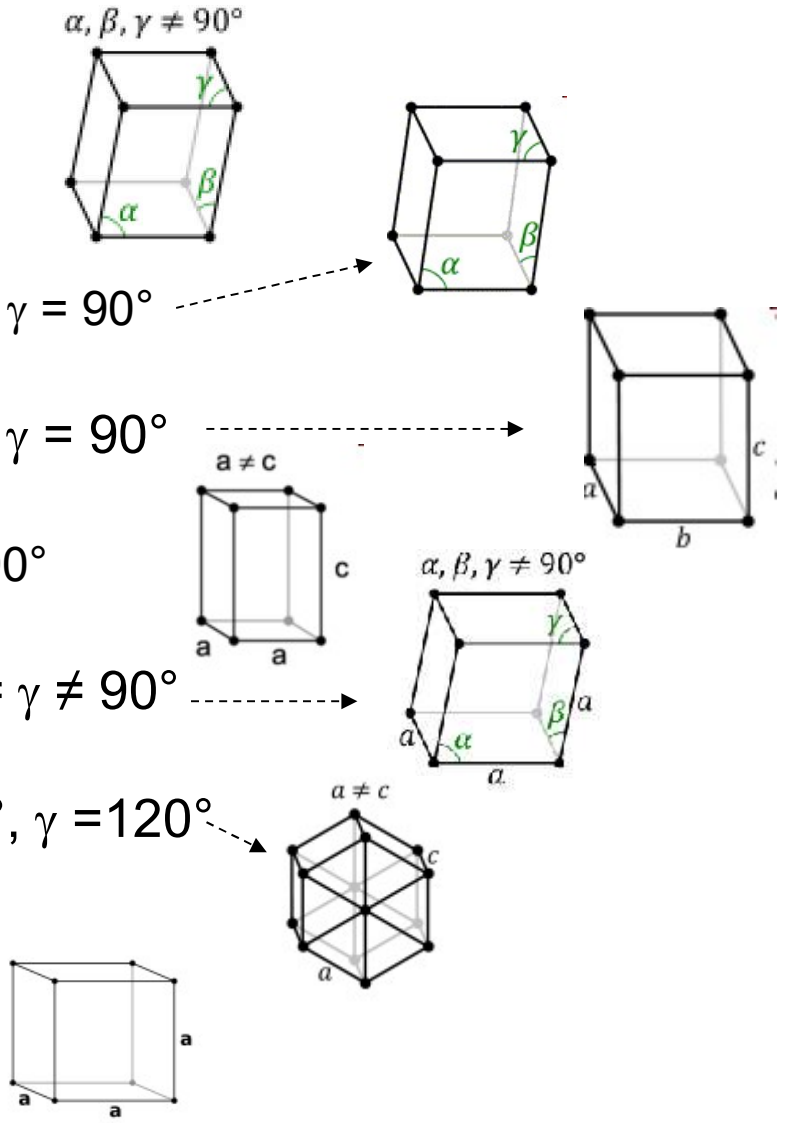
**orthorhombic:** a ≠ b ≠ c and $\alpha = \beta = \gamma = 90°$

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

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

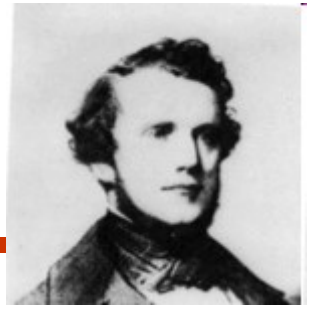
**hexagonal:** a = b ≠ c and $\alpha = \beta = 90°, \gamma = 120°$

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

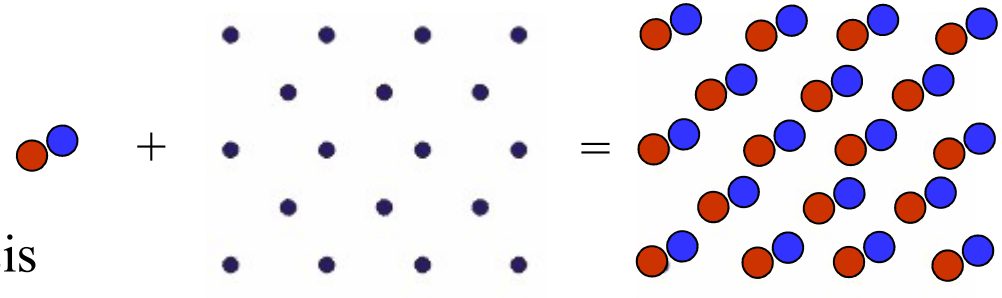



$\alpha$ is the angle between b and c

# Bravais lattice



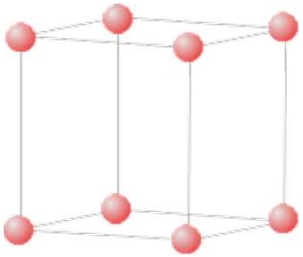
Auguste Bravais



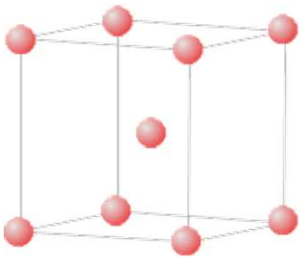

basis

Bravais lattice

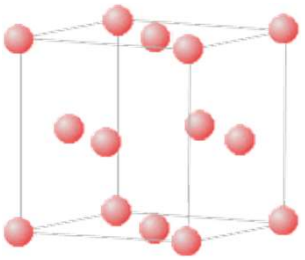
Crystal



simple cubic

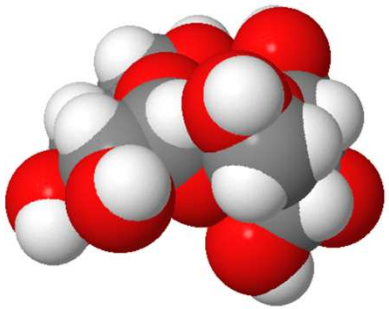


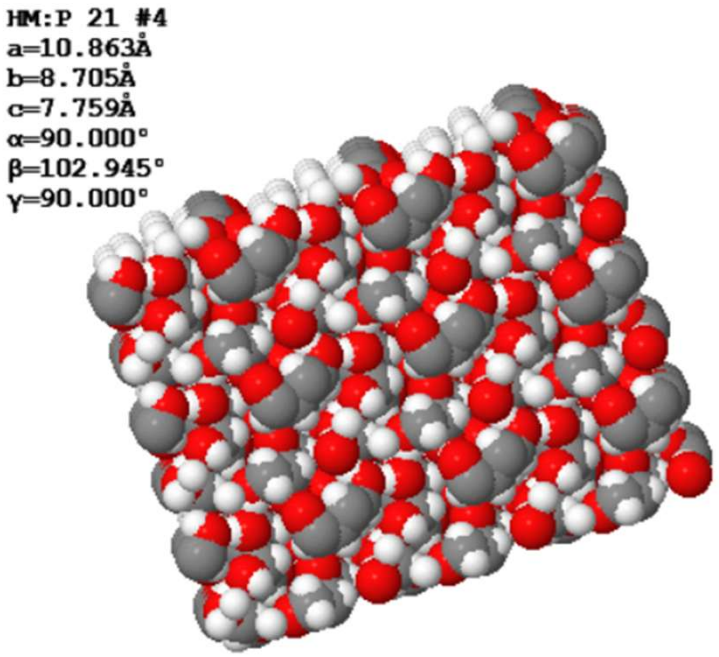
body centered cubic, bcc



face centered cubic, fcc

# Sugar (Sucrose)

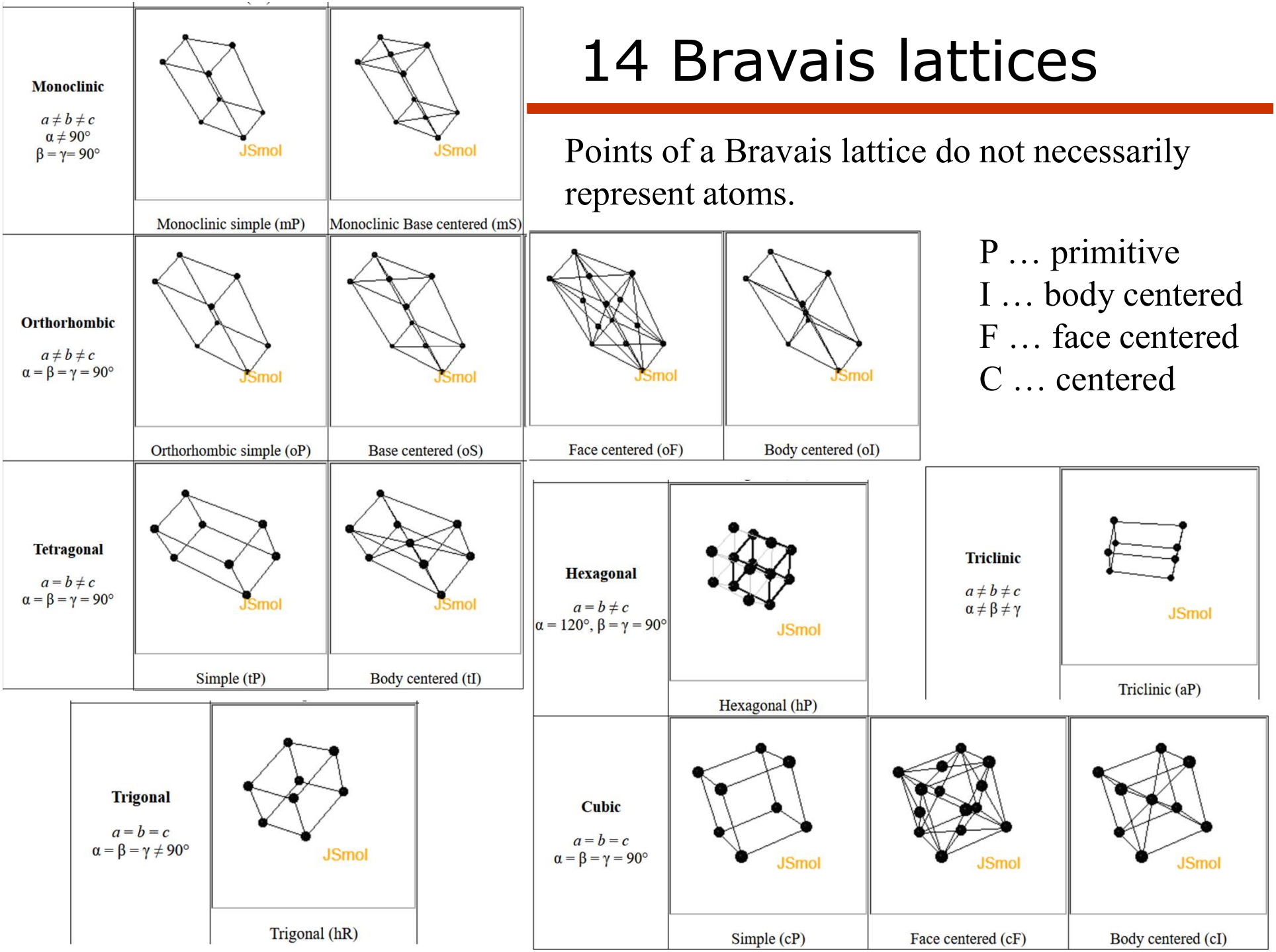




# 14 Bravais lattices

Points of a Bravais lattice do not necessarily represent atoms.

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

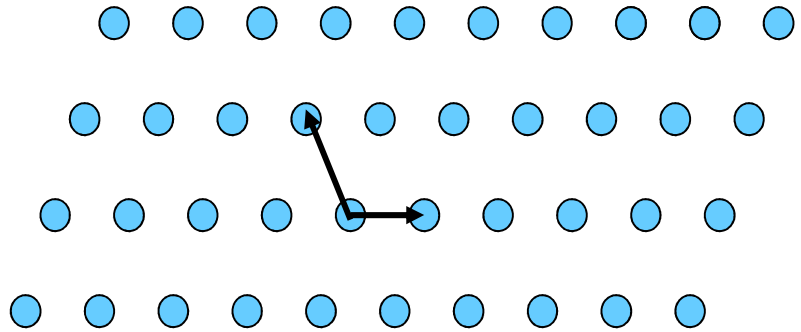


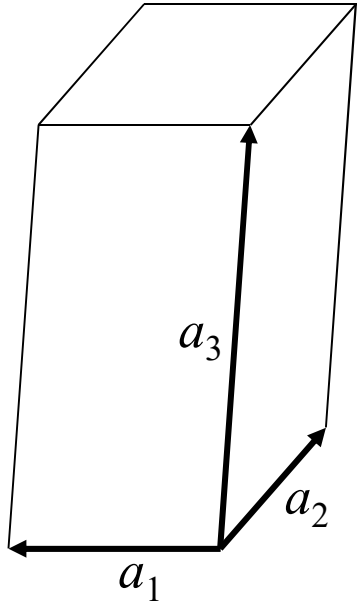
# Primitive lattice vectors

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

Translation vector

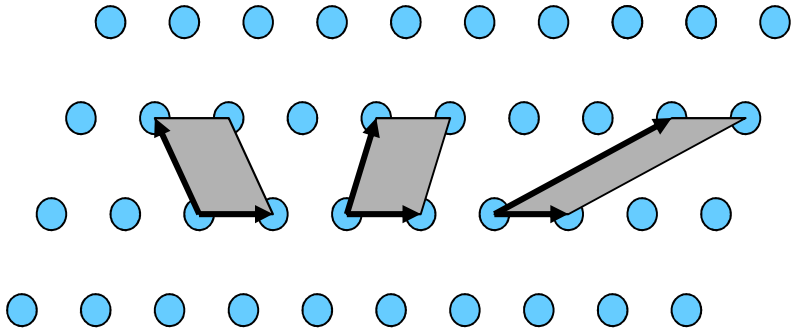
$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 = \cdots -2, -1, 0, 1, 2, \cdots$$



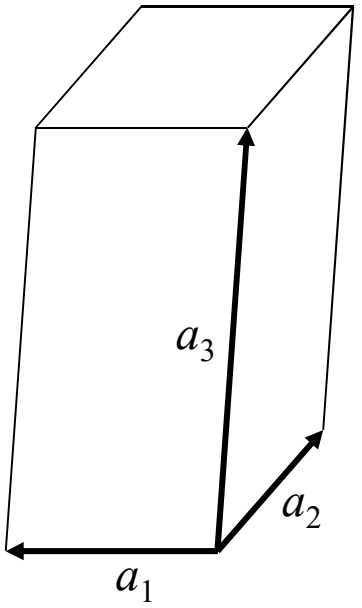



Primitive lattice vectors

# Primitive Unit Cell



There is more than one choice for a primitive unit cell




volume of a unit cell =

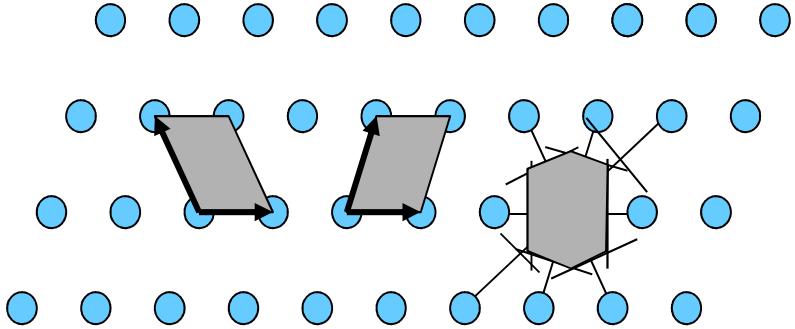
$$|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

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

There is more one primitive unit cell per Bravais lattice point.

# Unit Cells

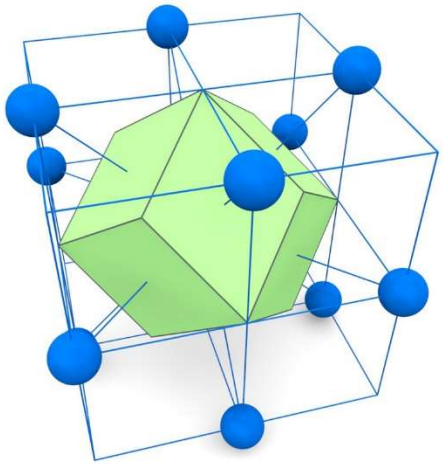
There is more than one choice for a primitive unit cell



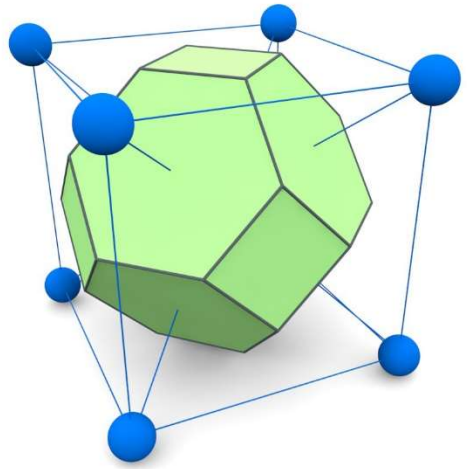
Eugene Wigner

Frederick Seitz

Wigner-Seitz primitive unit cell

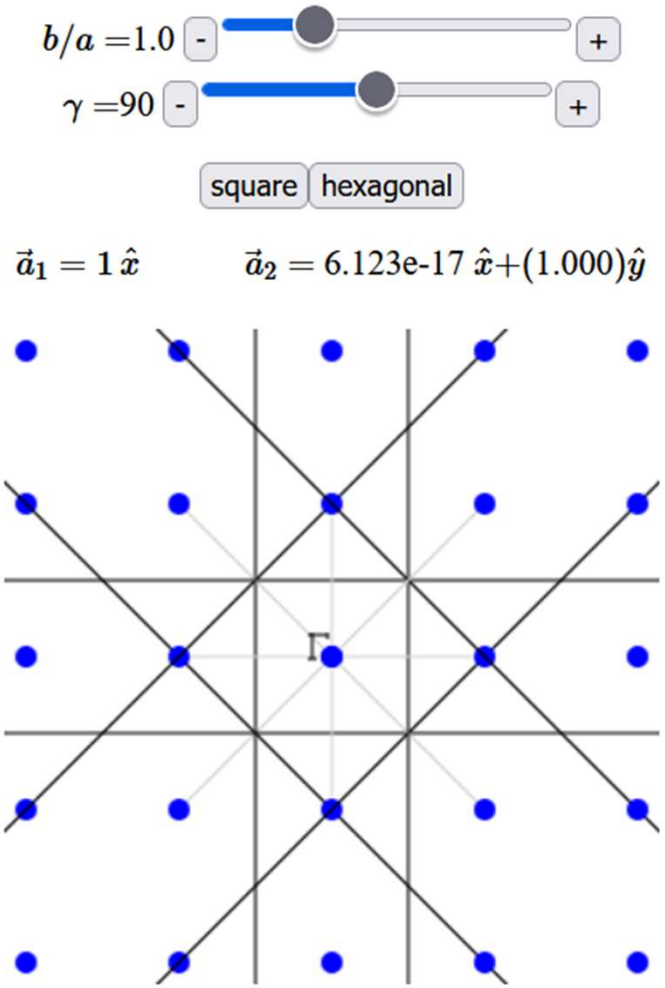


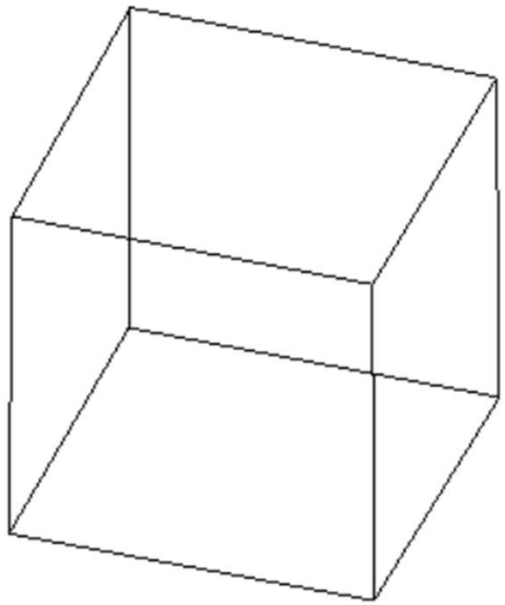
fcc



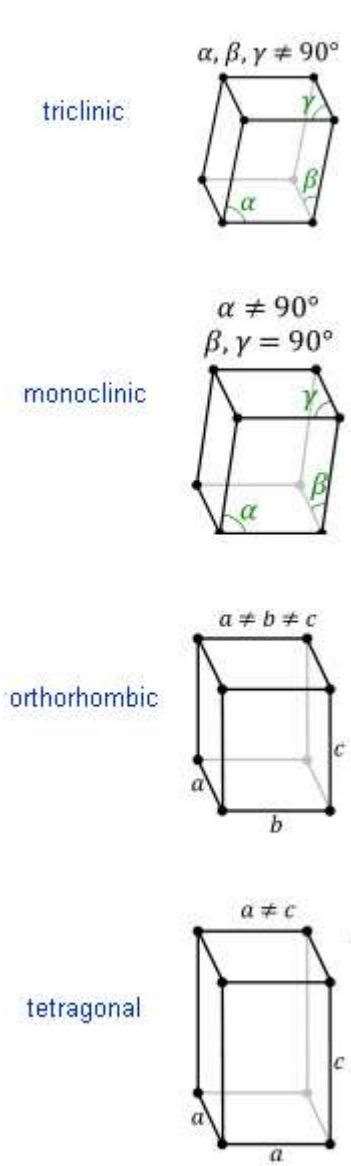
bcc

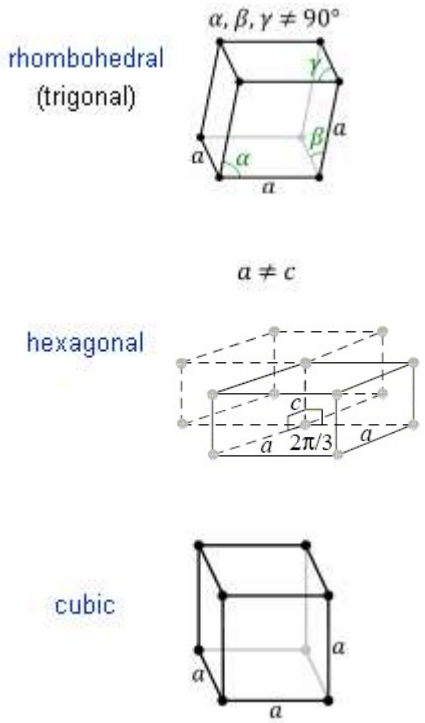
# Wigner-Seitz cells



# Conventional (crystallographic) unit cell



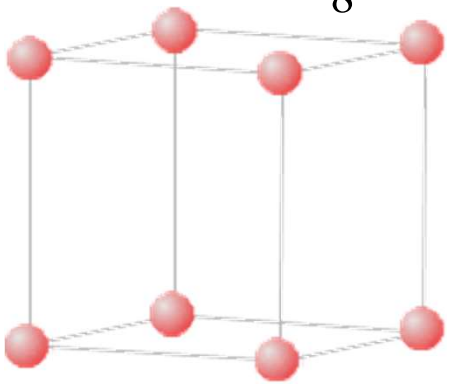

α is the angle between *b* and *c*
β is the angle between *a* and *c*
γ is the angle between *a* and *b*

6 faces, 8 corners

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

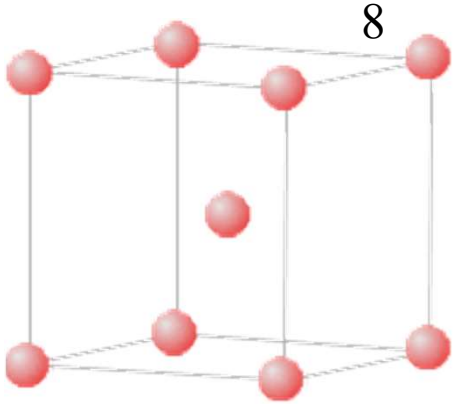
# Conventional (crystalographic) unit cell

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



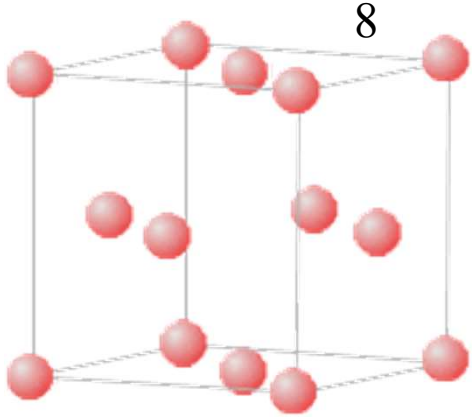
simple cubic

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

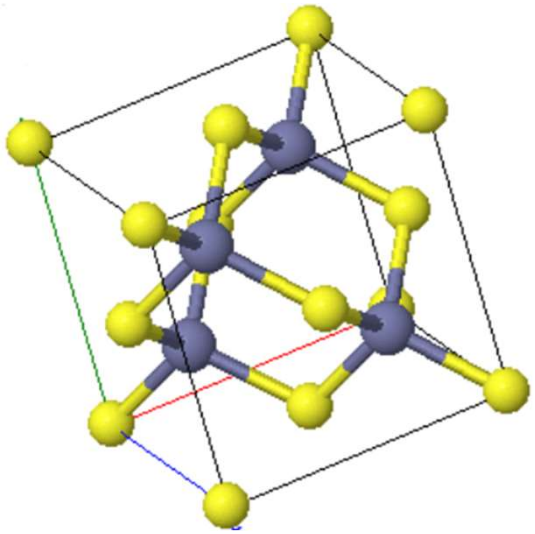


bcc

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

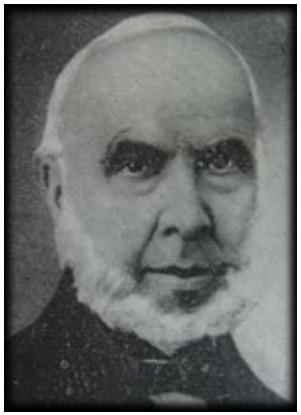


fcc



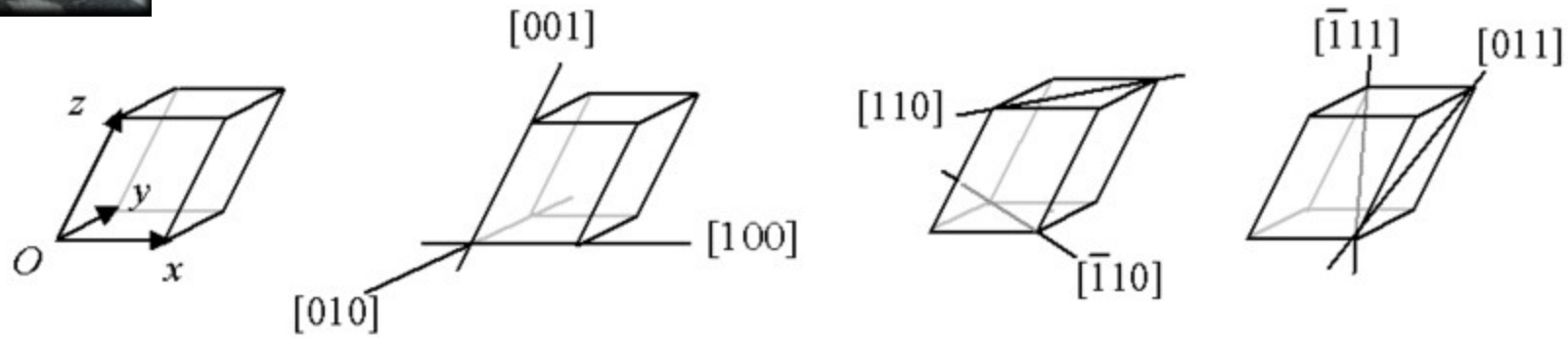
zincblende

# Miller indices: Crystal direction [*uvw*]



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

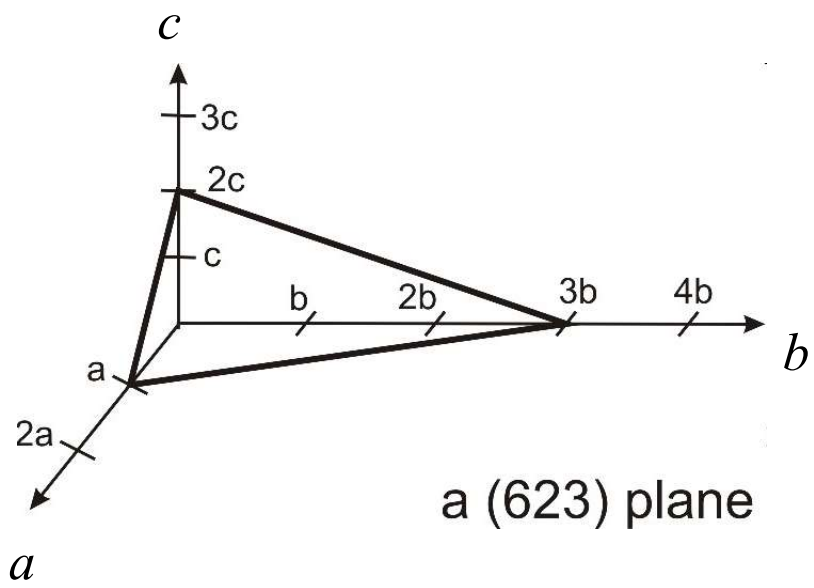
lattice vectors of the crystallographic unit cell




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

[ ] specific direction
< > family of equivalent directions

# Miller indices: Crystal planes



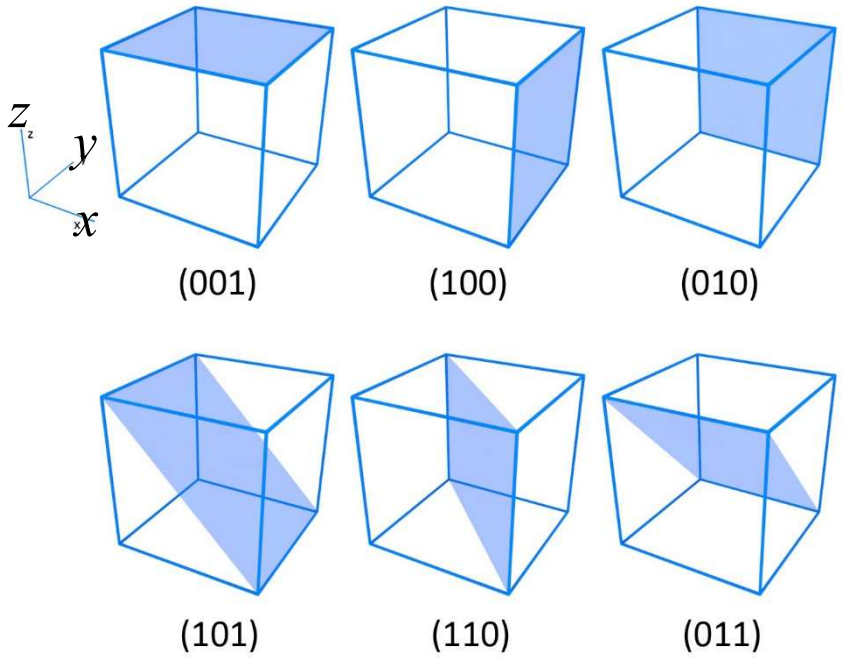

A plane with the intercepts $1/h, 1/k, 1/l$ is the $(h,k,l)$ plane.

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

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

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

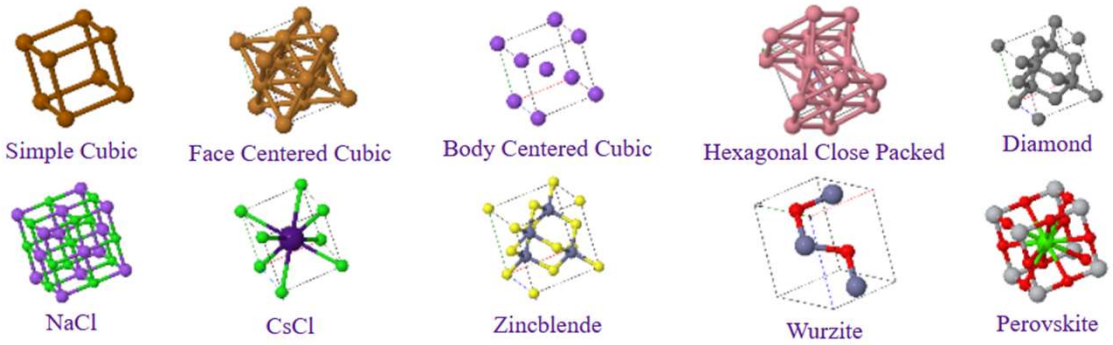
The length of the translation vector is, 4.12e-10 [m].

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

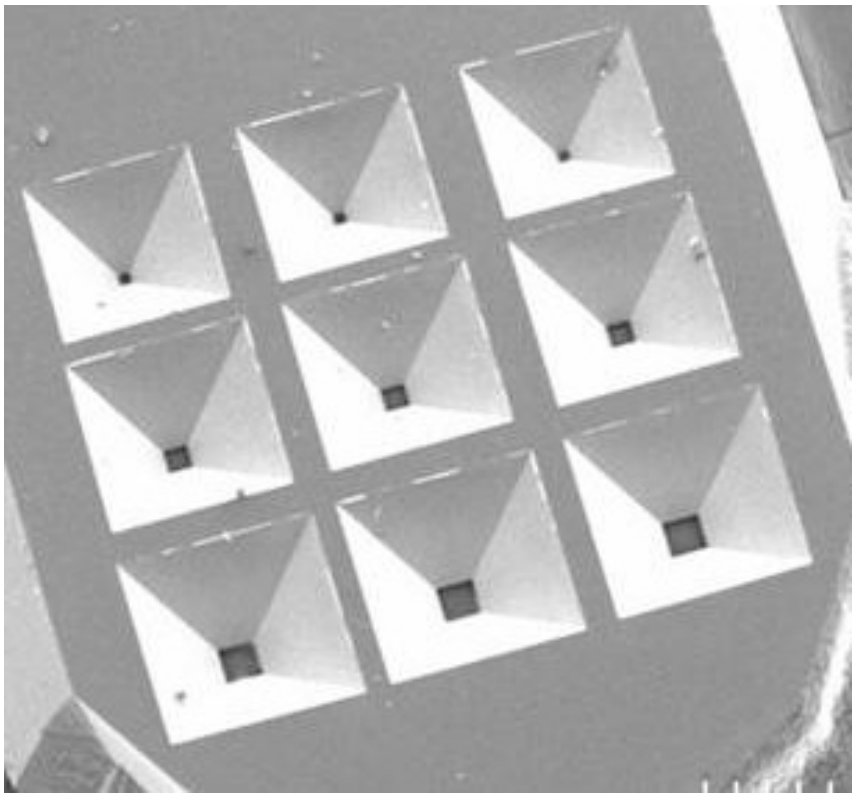
The unit vector in the $\vec{T}_{hkl}$ direction is, $\hat{T}_{hkl} =$ 1.00 $\hat{x}+$ 0.00 $\hat{y}+$ 0.00 $\hat{z}$.

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

ıw crystalographic planes of different crystal structures. The JSmol models of some common crystal structures are linked below.



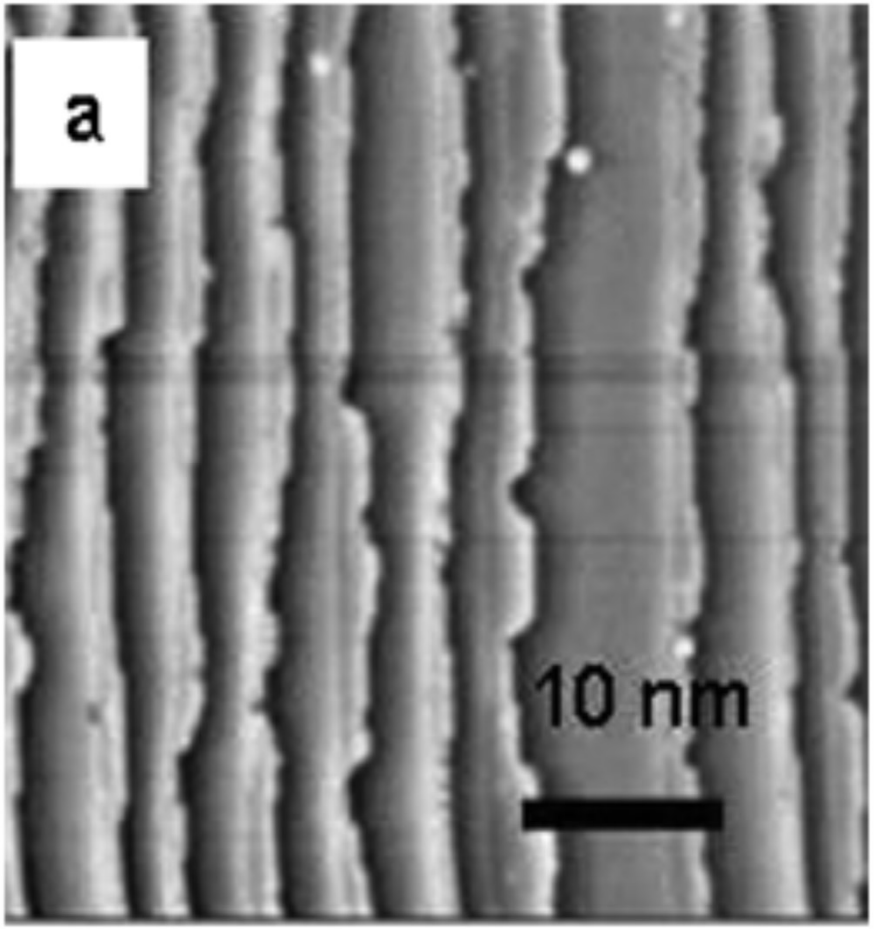
# KOH etching of silicon



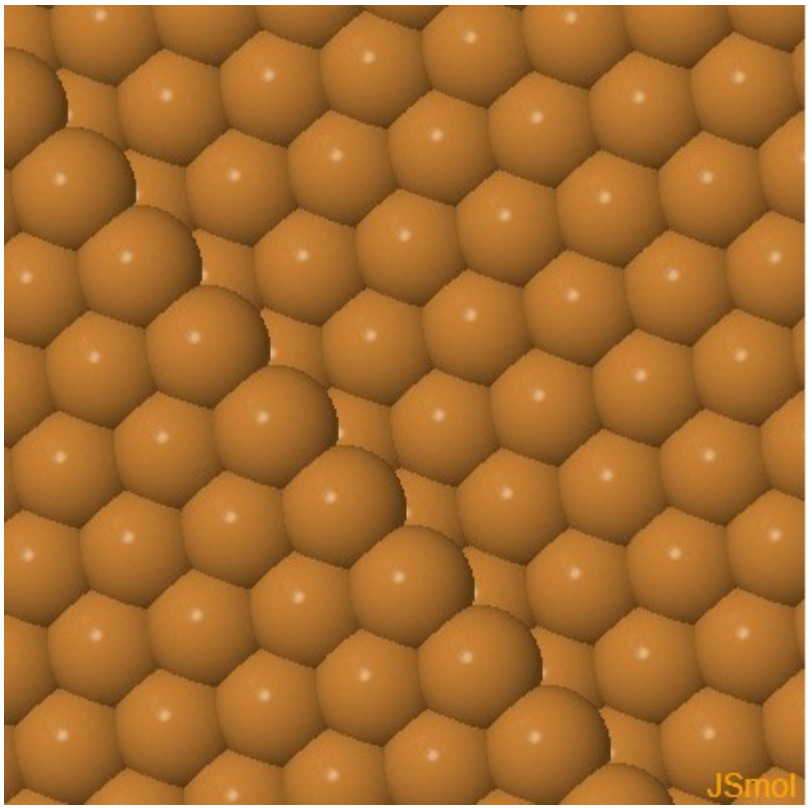
KOH etches Si {110} > {100} > {111}, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

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

# Crystal planes: Miller indices




Rh(15,15,13) fcc




(15,15,13) fcc

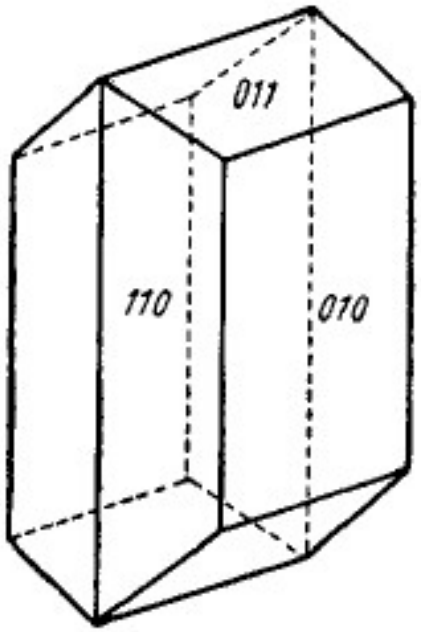
Reaction studies on nanostructured surfaces, Adolf Winkler, in *The Oxford Handbook of Nanoscience and Technology*, A. V. Narlikar and Y. Y. Fu ed., 2009.

# Crystals

**rule of rationality**

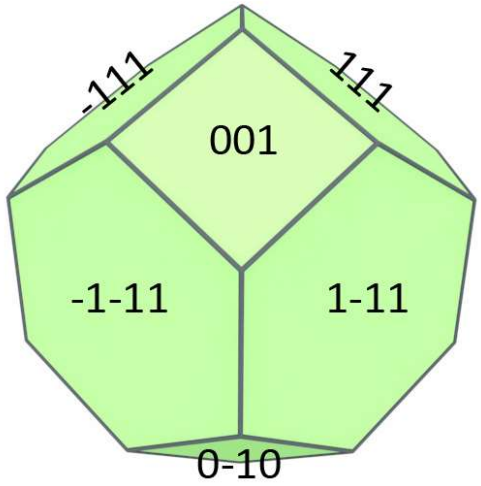
R. J. Haüy (1743-1822):

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

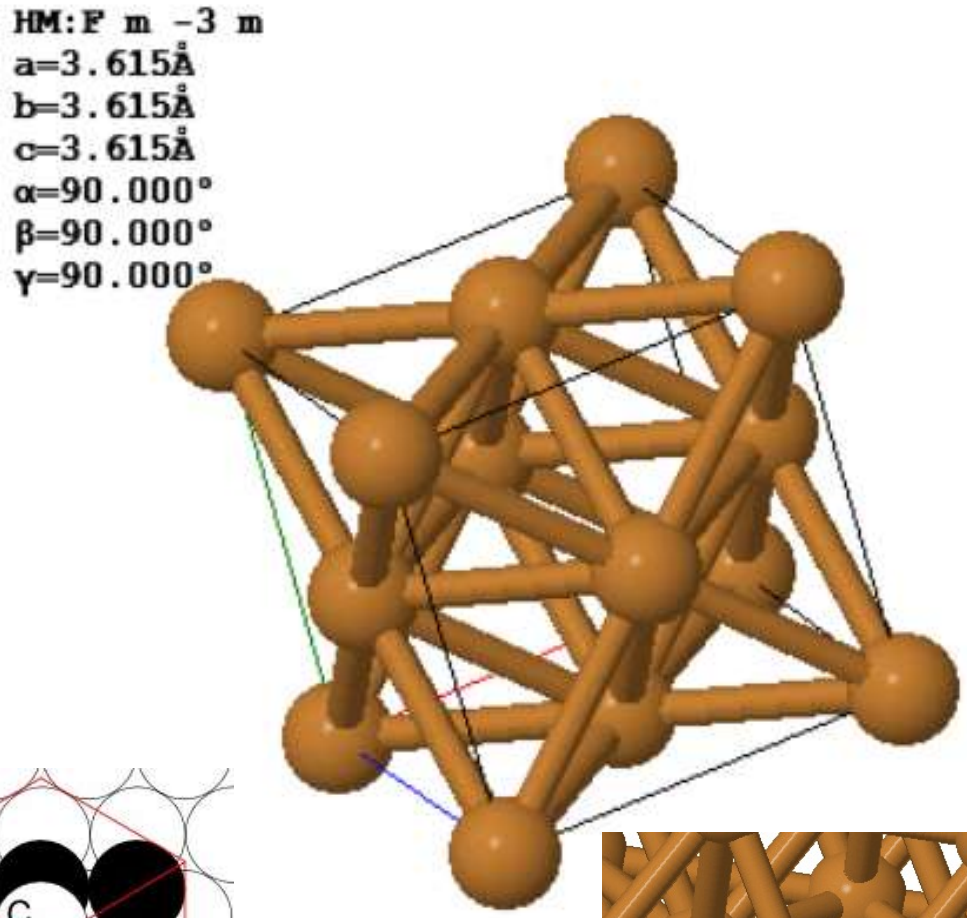
Bravais:

Planes with high atomic densities tend to dominate

# fcc

Number 225

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



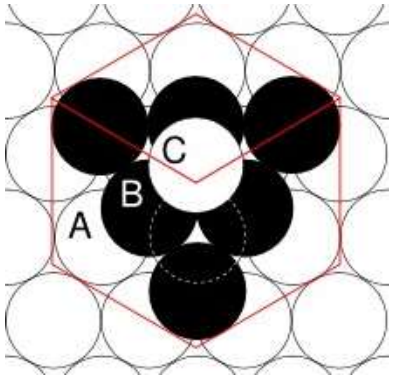

[111]

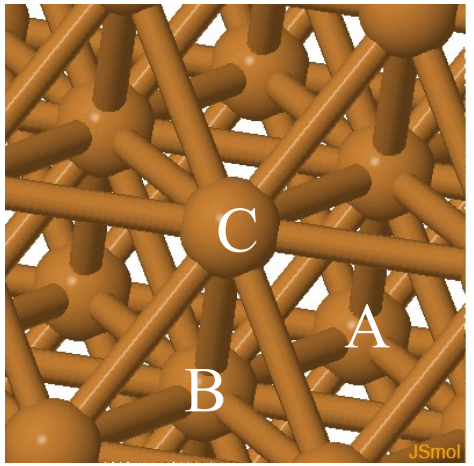
Primitive Vectors:

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

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

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




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