

# Introduction to Solid State Physics

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# Solid materials

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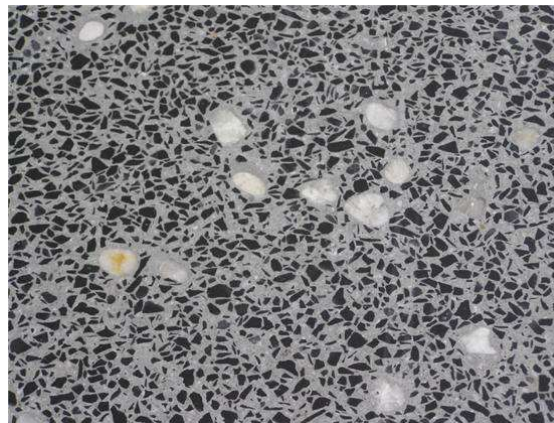
Metals and alloys

Plastics

Ceramics

Biological materials

Composite materials



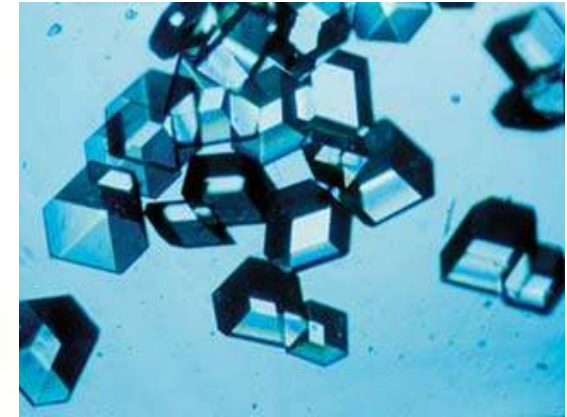
# Crystal = periodic arrangement of atoms



Gallium crystals



quartz



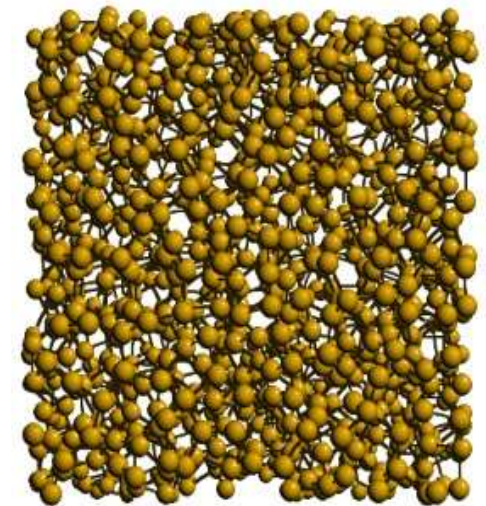
Insulin crystals



amorphous metal



glass



amorphous silicon

<http://www.wikipedia.org>

[http://www.pmc.umontreal.ca/~mousseau/site\\_an/uploads/Main/si1000.jpg](http://www.pmc.umontreal.ca/~mousseau/site_an/uploads/Main/si1000.jpg)

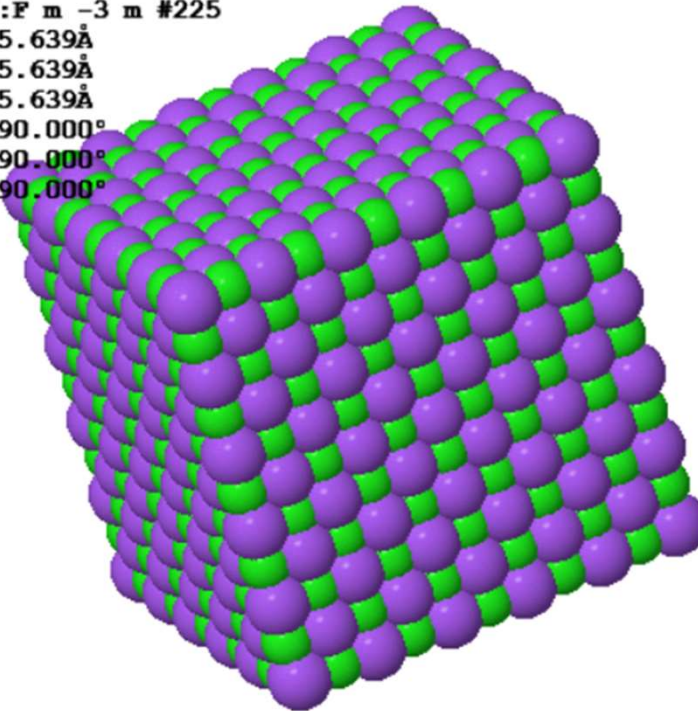


# Goal

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From the microscopic structure

HM: F m  $\bar{3}$  m #225  
a=5.639Å  
b=5.639Å  
c=5.639Å  
 $\alpha=90.000^\circ$   
 $\beta=90.000^\circ$   
 $\gamma=90.000^\circ$



calculate any property of any solid.

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



Print version

## MAS.020UF Introduction to Solid State Physics

### Course outline

Outline

Crystal Structure

Crystal Physics

Diffraction

Phonons

Exam questions

Appendices

Lectures

Books

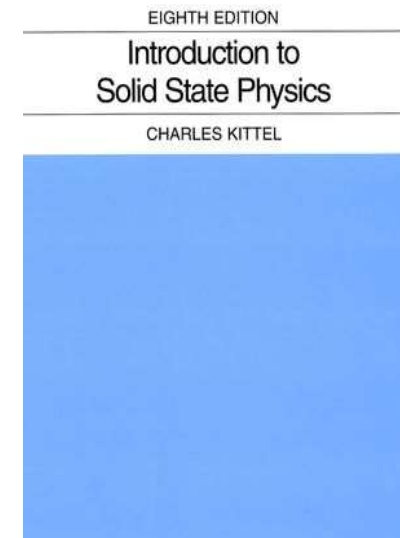
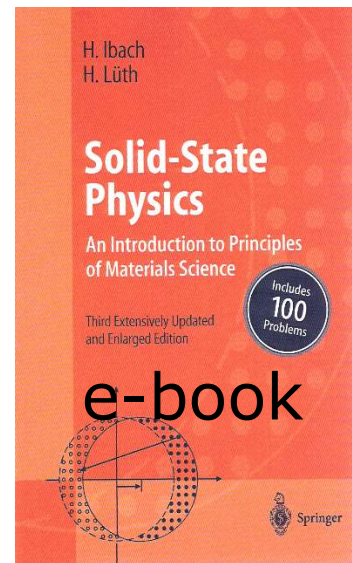
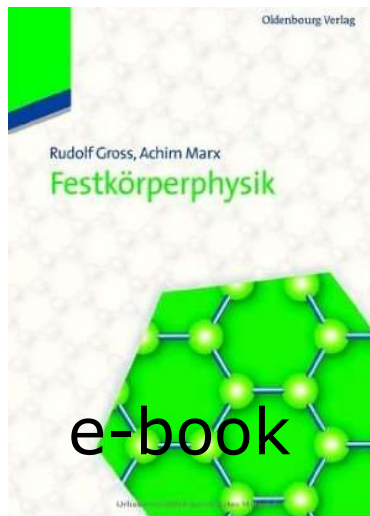
- **Crystal structure**

- 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, zinblende, 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

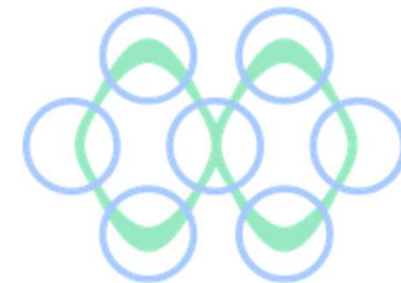
- **Crystal physics**

- SGTE data for pure elements - The Gibbs energy as a function of temperature for many

# Books



Inorganic Crystal Structure Database



Materials Project

# Carbon polytypes

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Different polytypes  $\Rightarrow$  Different properties

# Aluminum and Silicon

## Conductivity

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

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

10.81	12.01	14.01
13	14	15
Al	Si	P
26.98	28.09	30.97
31	32	33

atomic mass [amu]      1      266

**Atomic Mass**

1 amu = 1.66054 × 10<sup>-27</sup> kg

1																	2				
H 1.008																	He 4.003				
3	4															5	6	7	8	9	10
Li 6.941	Be 9.012															B 10.81	C 12.01	N 14.01	O 16	F 19	Ne 20.18
11	12															13	14	15	16	17	18
Na 22.99	Mg 24.31															Al 26.98	Si 28.09	P 30.97	S 32.07	Cl 35.45	Ar 39.95
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36				
K 39.1	Ca 40.08	Sc 44.96	Ti 47.88	V 50.94	Cr 52	Mn 54.94	Fe 55.85	Co 58.47	Ni 58.69	Cu 63.55	Zn 65.39	Ga 69.72	Ge 72.59	As 74.92	Se 78.96	Br 79.9	Kr 83.8				
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54				
Rb 85.47	Sr 87.62	Y 88.91	Zr 91.22	Nb 92.91	Mo 95.94	Tc 98	Ru 101.1	Rh 102.9	Pd 106.4	Ag 107.9	Cd 112.4	In 114.8	Sn 118.7	Sb 121.8	Te 127.6	I 126.9	Xe 131.3				
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86				
Cs 132.9	Ba 137.3	La 138.9	Hf 178.5	Ta 180.9	W 183.9	Re 186.2	Os 190.2	Ir 190.2	Pt 195.1	Au 197	Hg 200.5	Tl 204.4	Pb 207.2	Bi 209	Po 210	At 210	Rn 222				
87	88	89	104	105	106	107	108	109													
Fr 223	Ra 226	Ac 227	Rf 257	Db 260	Sg 263	Bh 262	Hs 265	Mt 266													
58	59	60	61	62	63	64	65	66	67	68	69	70	71								
Ce 140.1	Pr 140.9	Nd 144.2	Pm 147	Sm 150.4	Eu 152	Gd 157.3	Tb 158.9	Dy 162.5	Ho 164.9	Er 167.3	Tm 168.9	Yb 173	Lu 175								
90	91	92	93	94	95	96	97	98	99	100	101	102	103								
Th 232	Pa 231	U 238	Np 237	Pu 242	Am 243	Cm 247	Bk 247	Cf 249	Es 254	Fm 253	Md 256	No 254	Lr 257								



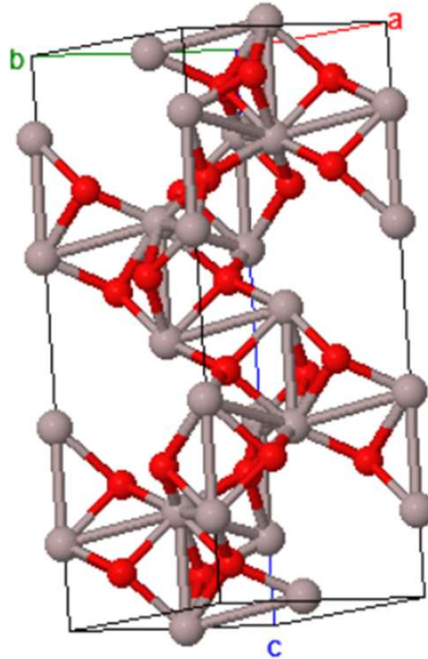
# Sapphire and Ruby

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Ti

HM:R -3 c #167  
a=4.757Å  
b=4.757Å  
c=12.988Å  
α=90.000°  
β=90.000°  
γ=120.000°



$\text{Al}_2\text{O}_3$



Cr

[https://en.wikipedia.org/wiki/Ruby#/media/File:Ruby\\_gem.JPG](https://en.wikipedia.org/wiki/Ruby#/media/File:Ruby_gem.JPG)

[https://en.wikipedia.org/wiki/Sapphire#/media/File:Geschliffener\\_blauer\\_Saphir.jpg](https://en.wikipedia.org/wiki/Sapphire#/media/File:Geschliffener_blauer_Saphir.jpg)

# 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**

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

Implementation **7 x 90 min :**

**Data to be decided via doodle**

**<https://doodle.com/meeting/participate/id/e15lyA7a>**

***Mandatory Presence!***



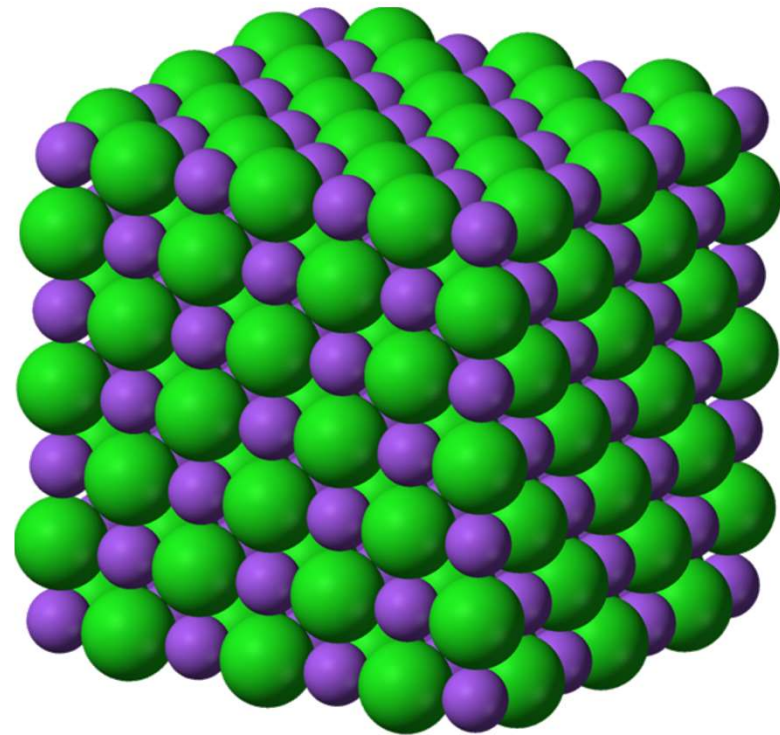
# Crystal structure

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# Crystal structure

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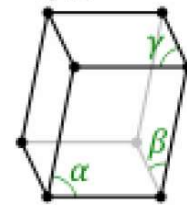
A crystal is a three dimensional periodic arrangement of atoms.



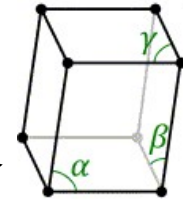
# 7 Crystal Systems

**triclinic:**  $a \neq b \neq c$  and  $\alpha \neq \beta \neq \gamma \neq 90^\circ$

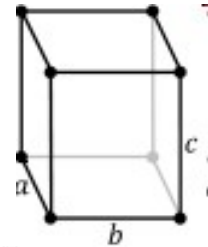
$\alpha, \beta, \gamma \neq 90^\circ$



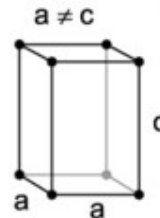
**monoclinic:**  $a \neq b \neq c$  and  $\alpha \neq 90^\circ$   $\beta = \gamma = 90^\circ$



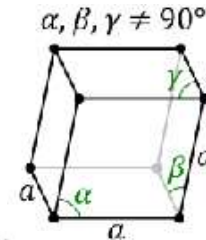
**orthorhombic:**  $a \neq b \neq c$  and  $\alpha = \beta = \gamma = 90^\circ$



**tetragonal:**  $a = b \neq c$  and  $\alpha = \beta = \gamma = 90^\circ$



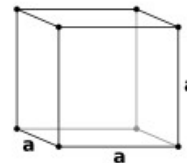
**rhombohedral:**  $a = b = c$  and  $\alpha \neq \beta \neq \gamma \neq 90^\circ$



**hexagonal:**  $a = b \neq c$  and  $\alpha = \beta = 90^\circ$ ,  $\gamma = 120^\circ$

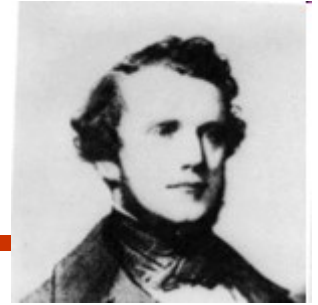


**cubic**  $a = b = c$  and  $\alpha = \beta = \gamma = 90^\circ$

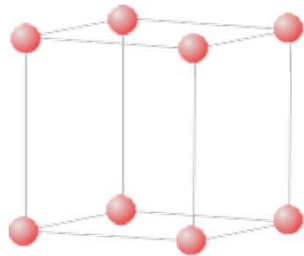
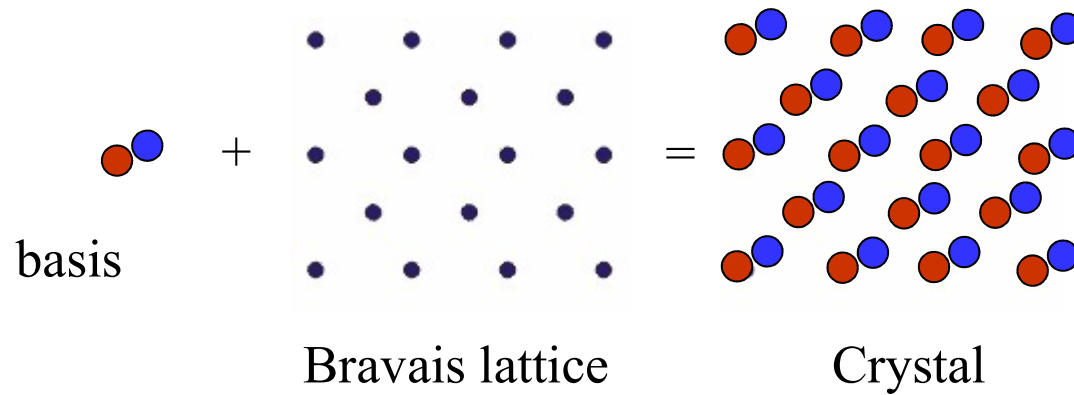


$\alpha$  is the angle between b and c

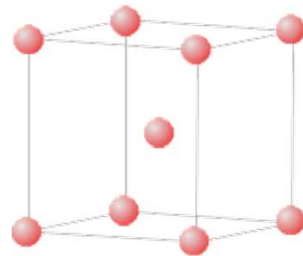
# Bravais lattice



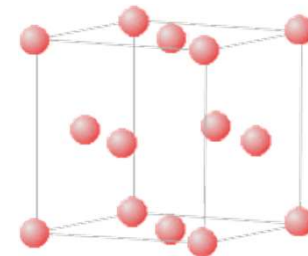
Auguste Bravais



simple cubic



body centered  
cubic, bcc



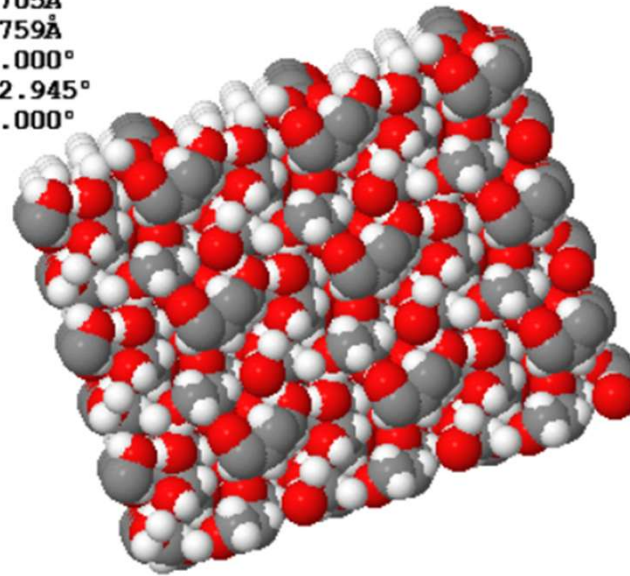
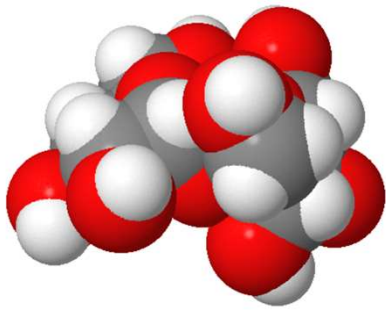
face centered  
cubic, fcc



# Sugar (Sucrose)

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HM:P 21 #4  
a=10.863Å  
b=8.705Å  
c=7.759Å  
 $\alpha=90.000^\circ$   
 $\beta=102.945^\circ$   
 $\gamma=90.000^\circ$



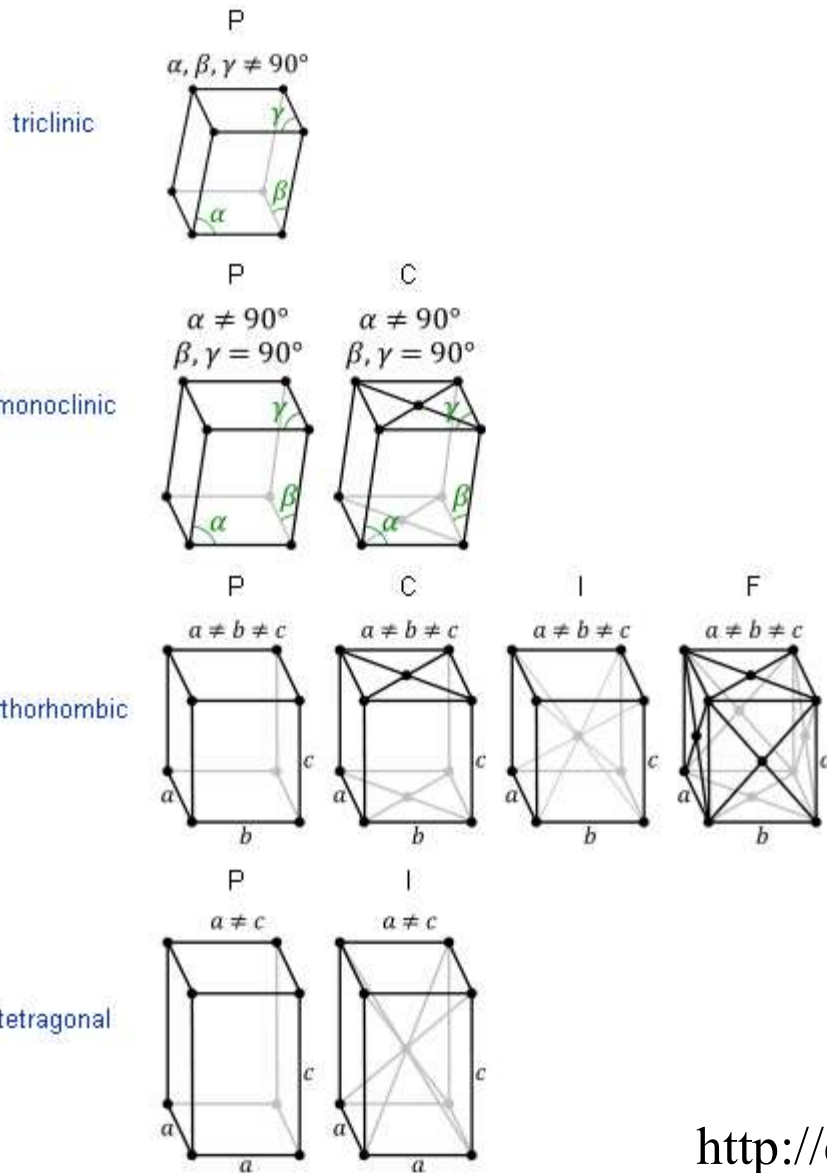
# 14 Bravais lattices

Crystal system

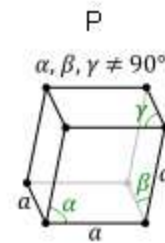
Bravais lattices

Crystal system

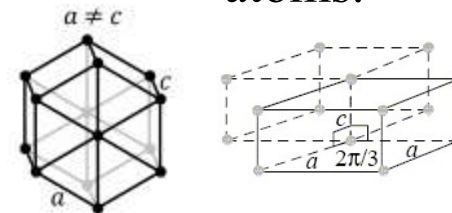
Bravais lattices



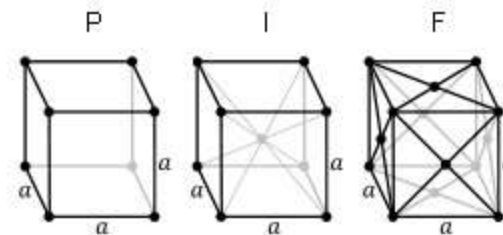
rhombohedral (trigonal)



hexagonal



cubic



Points of a Bravais lattice do not necessarily represent atoms.

- P ... primitive
- I ... body centered
- F ... face centered
- C ... centered

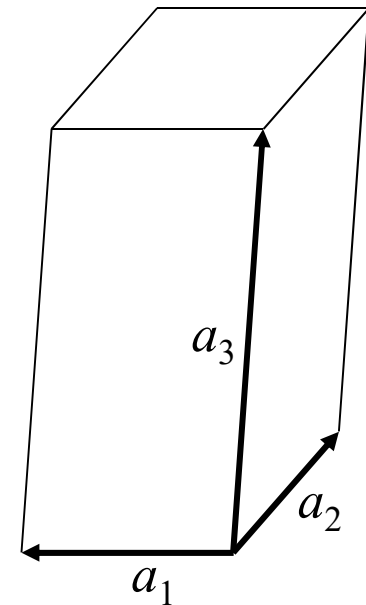
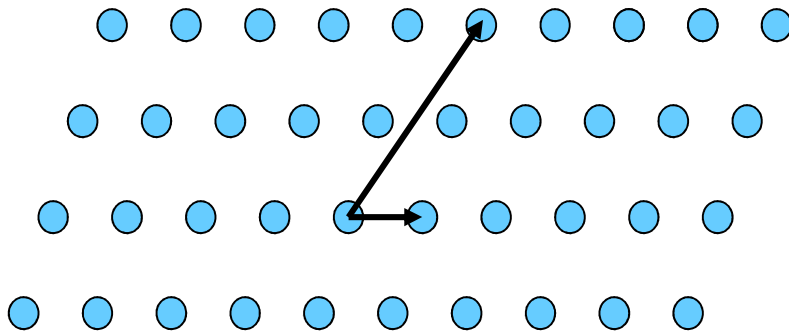
# Primitive lattice vectors

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

Translation vector

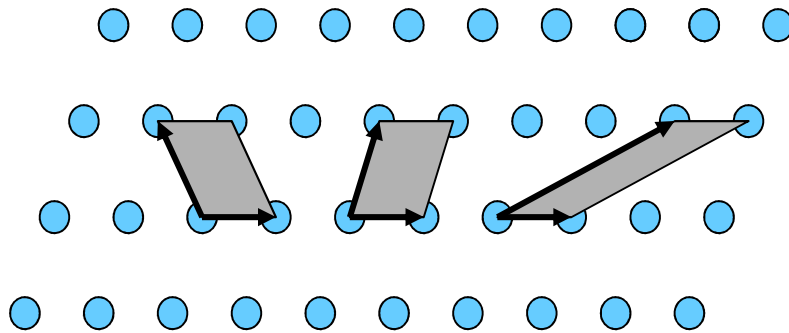
$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad n_1, n_2, n_3 = \dots -2, -1, 0, 1, 2, \dots$$



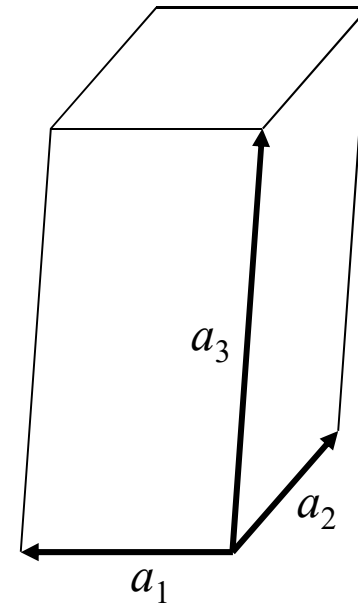
Primitive lattice vectors

# Primitive Unit Cell

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There is more than one choice for a primitive unit cell



volume of a unit cell =

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

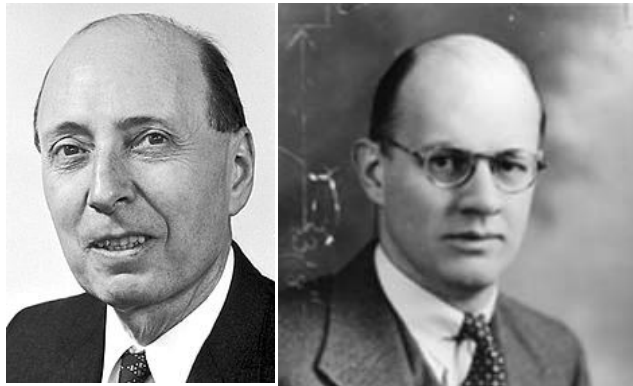
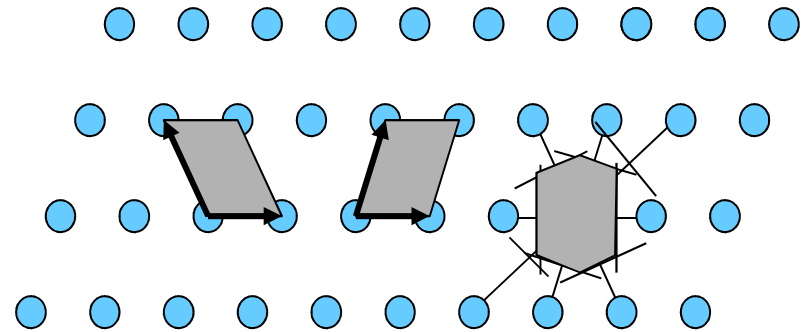
$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad n_1, n_2, n_3 = \dots -2, -1, 0, 1, 2, \dots$$



# Unit Cells

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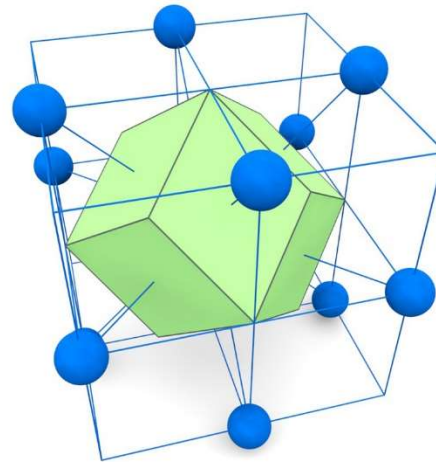
There is more than one choice for a primitive unit cell



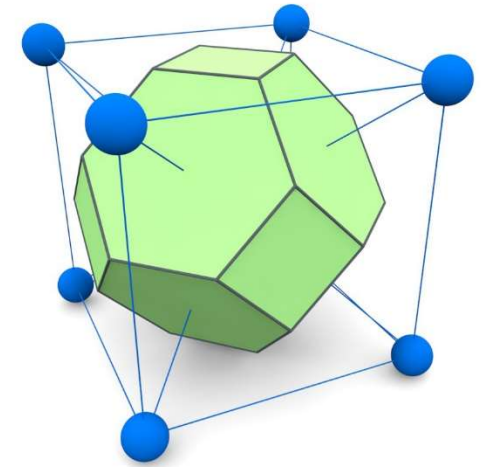
Eugene  
Wigner

Frederick  
Seitz

Wigner-Seitz primitive unit cell

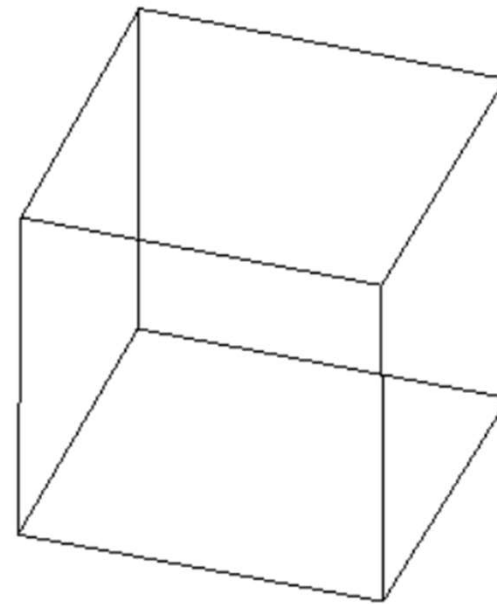
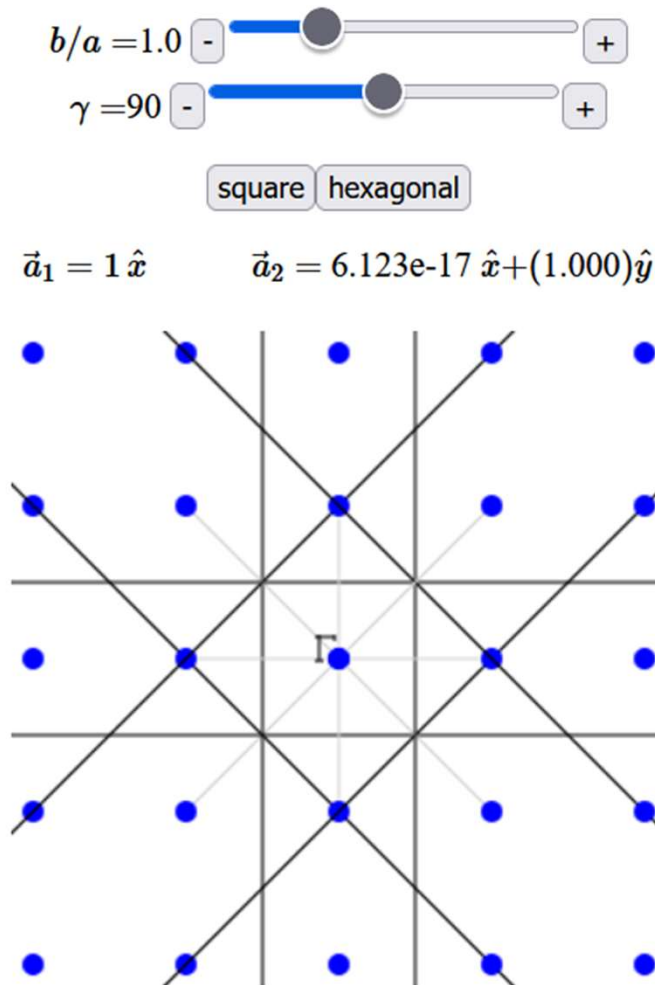


fcc

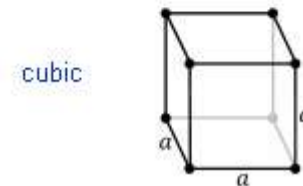
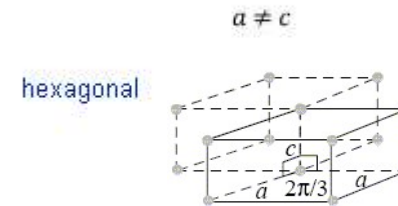
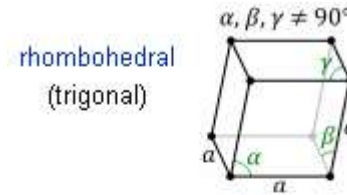
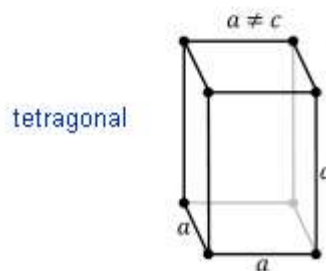
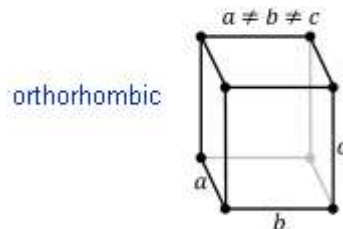
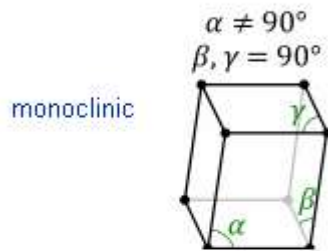
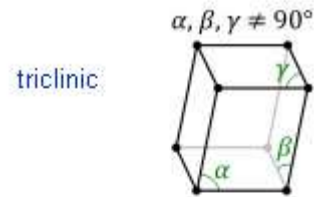


bcc

# Wigner-Seitz cells



# Conventional (crystallographic) unit cell



$\alpha$  is the angle between  $b$  and  $c$   
 $\beta$  is the angle between  $a$  and  $c$   
 $\gamma$  is the angle between  $a$  and  $b$

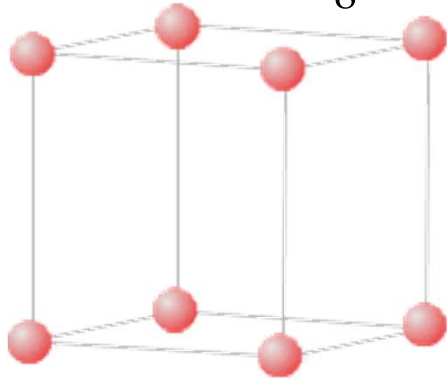
6 faces, 8 corners

[http://en.wikipedia.org/wiki/Bravais\\_lattice](http://en.wikipedia.org/wiki/Bravais_lattice)

# Conventional (crystallographic) unit cell

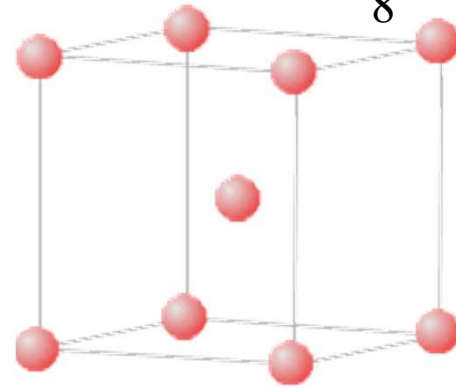
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$$8 \times \frac{1}{8} = 1$$



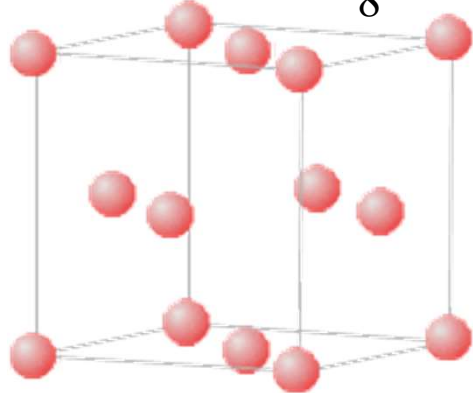
simple cubic

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

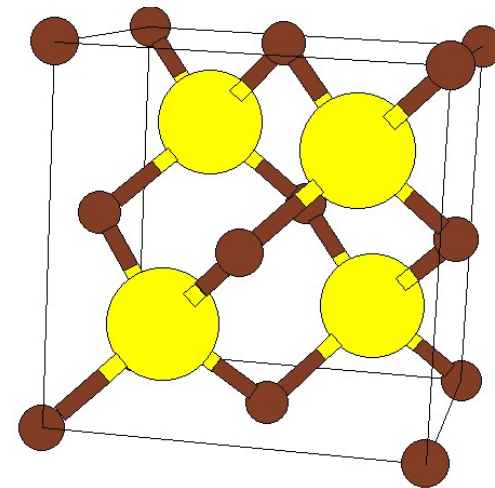


bcc

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



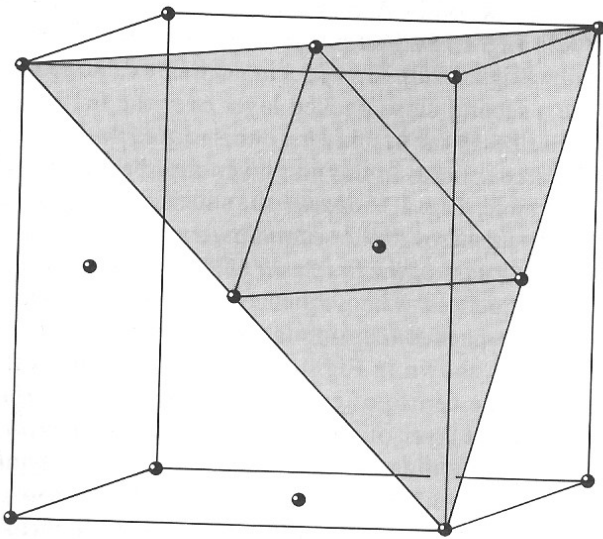
fcc



zincblende

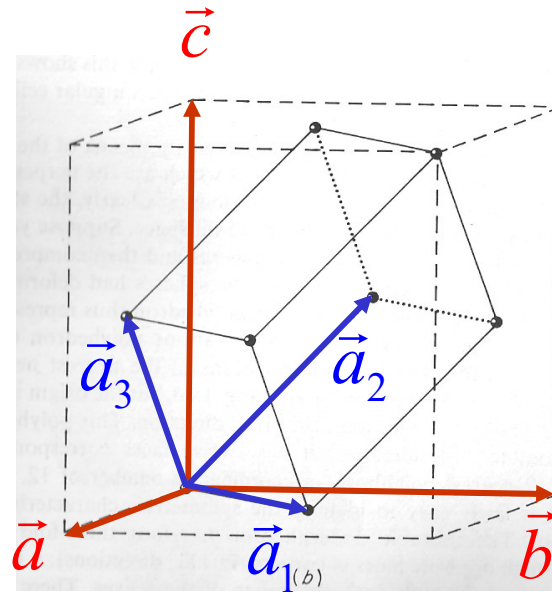
# Fcc

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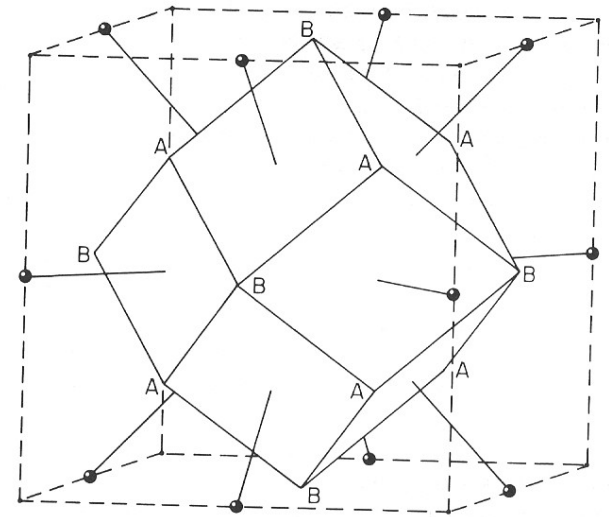


(a)

Crystallographic unit cell  
showing close packed  
plane



Crystallographic lattice  
vectors  
Primitive lattice vectors



Wigner-Seitz cell

From: Hall, Solid State Physics