

# M. Sc. Bionics Engineering



UNIVERSITÀ DI PISA



Sant'Anna  
Scuola Universitaria Superiore Pisa



SCUOLA  
ALTI STUDI  
LUCCA

## ADVANCED MATERIALS FOR BIONICS

## LECTURE 3: MATERIALS STRUCTURE 2

CRYSTAL STRUCTURE OF SOLIDS

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AY 2024-25

L3 - 04.10.2024, 07.10.2024



# QUESTIONS

- What is the difference in atomic arrangement between **crystalline** and **noncrystalline** solids?
- What are the crystal structures of metals?
- What are the characteristics of crystal structures?
- How are crystallographic points, directions, and planes specified?
- What characteristics of a material's atomic structure determine its density?
- How to determine a crystal structure?

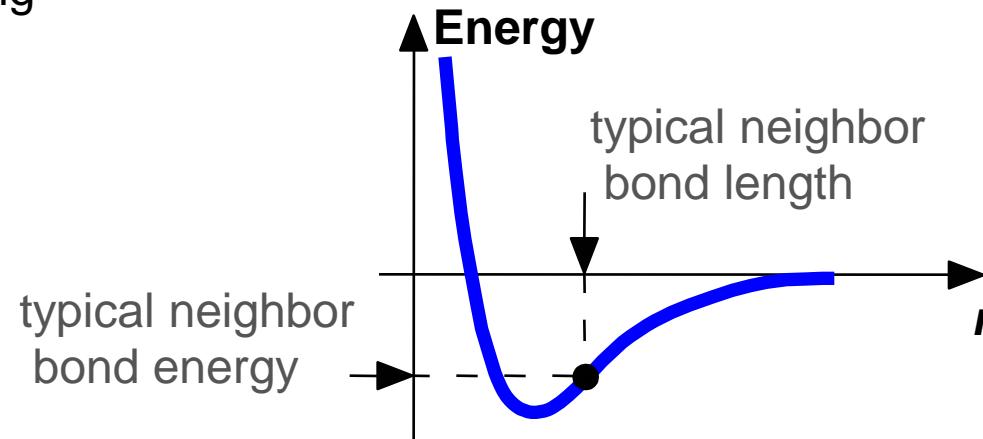
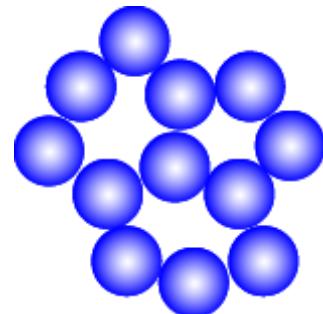


L3.1

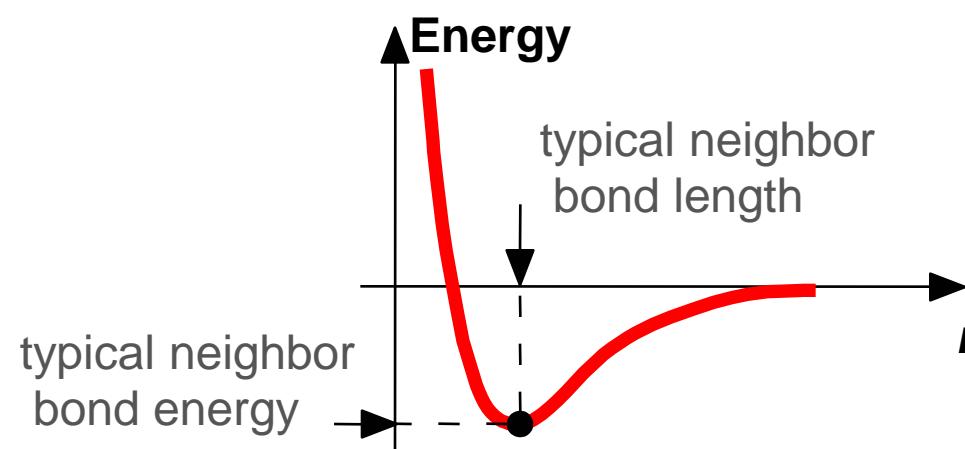
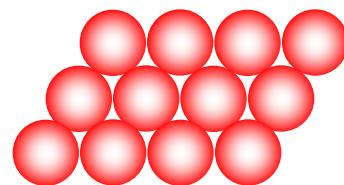
# CRYSTALLINE SOLIDS, DEFINITIONS

# ENERGY AND PACKING

- Non dense, **random** packing



- Dense, **ordered** packing

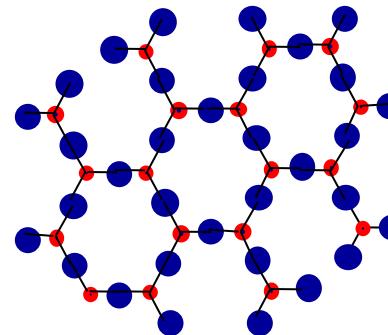


Ordered structures tend to be nearer the minimum in bonding energy and are more stable.

# MATERIALS AND ATOMIC ARRANGEMENTS

## Crystalline materials...

- atoms arranged in ordered, periodic, 3D lattice
- typical of:
  - metals
  - many ceramics
  - some polymers



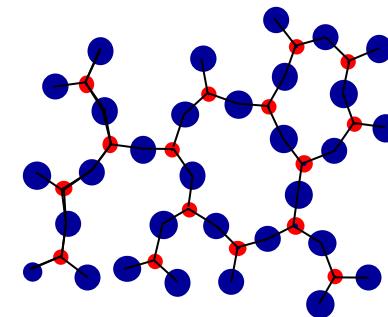
crystalline  $\text{SiO}_2$  (quartz)

Adapted from Fig. 3.24(a),  
*Callister & Rethwisch 10e.*

## Noncrystalline materials...

- atoms have no periodic arrangement
- occurs for:
  - complex structures
  - rapid cooling

• Si      • Oxygen

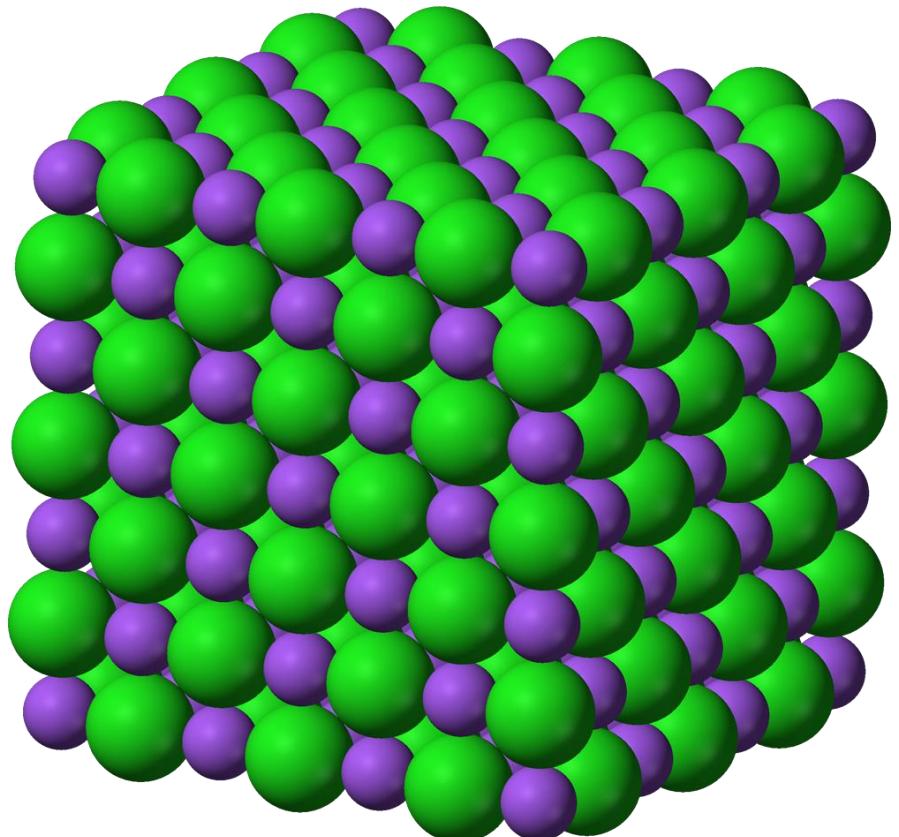


noncrystalline  $\text{SiO}_2$  (glass)

Adapted from Fig. 3.24(b),  
*Callister & Rethwisch 10e.*

"Amorphous" = Noncrystalline

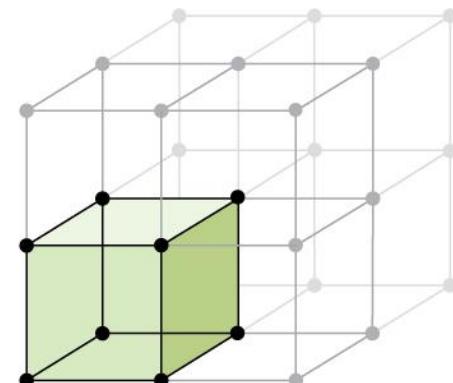
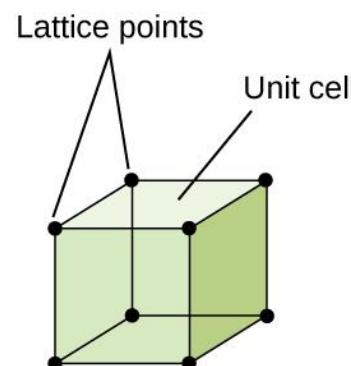
# CRYSTAL



# CRYSTAL STRUCTURES

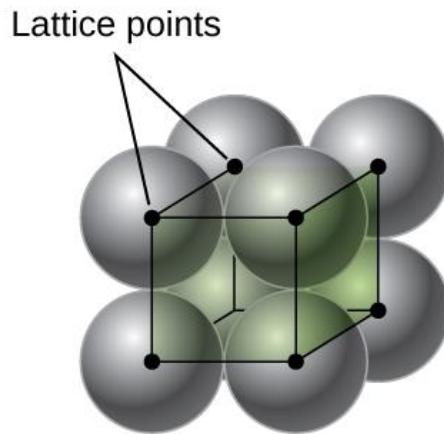
in crystals a **unit cell** (tile) contains all the atoms of a compound and its repetition (lattice) creates an «infinite» structure

**Unit cell:** smallest repeating unit of the periodic lattice

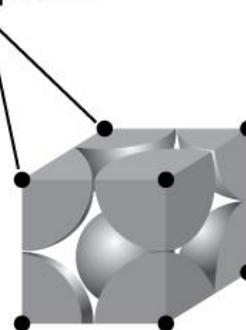


simple cubic  
(SC)

Example:  
1 atom per unit cell



Simple cubic lattice cell

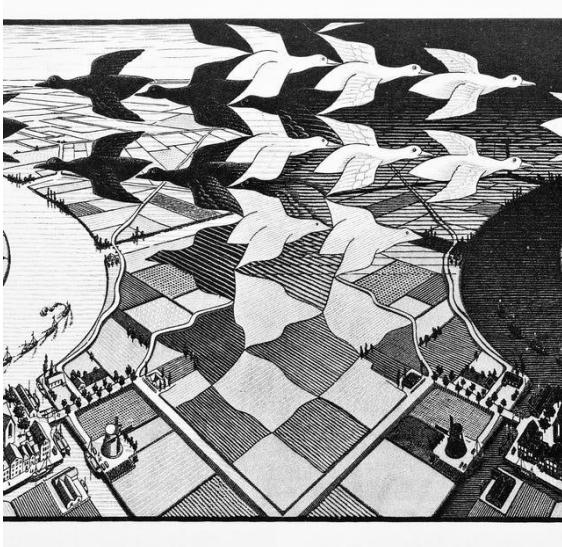
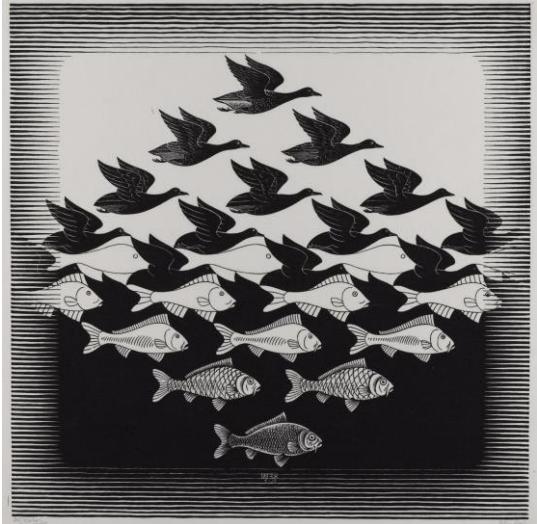


8 corners

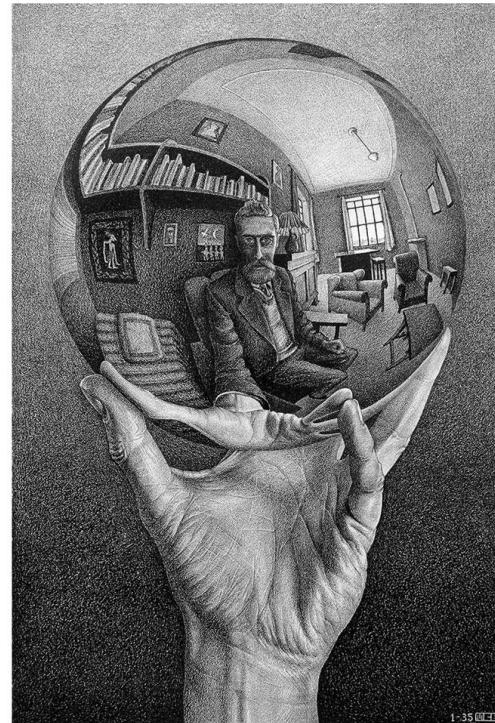
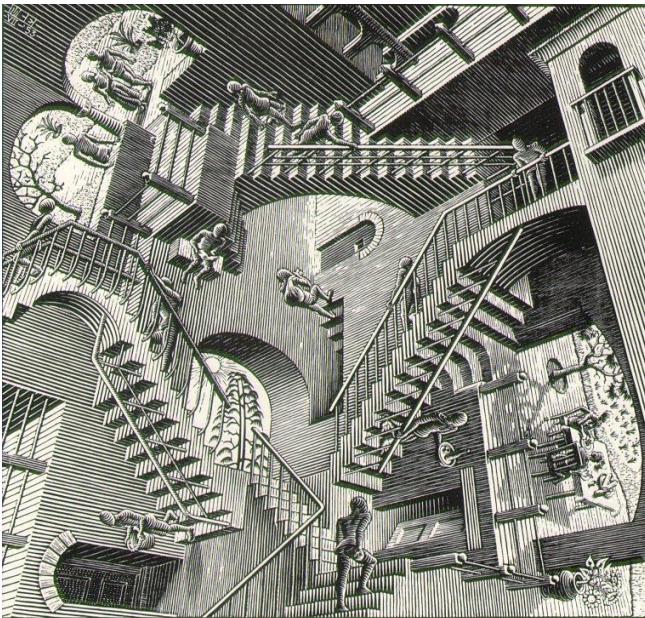
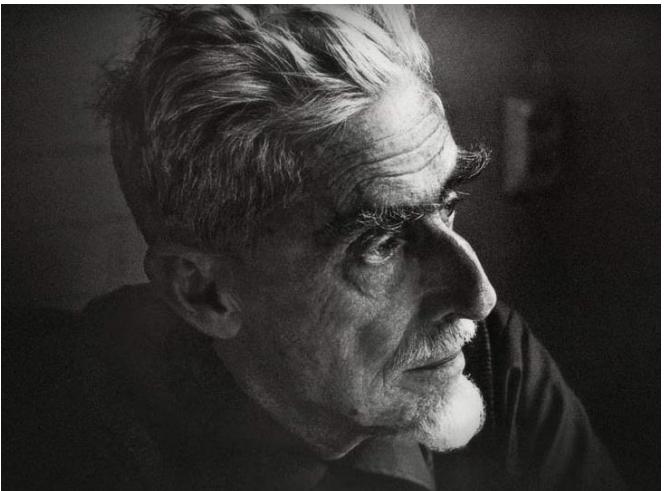


L3.2

# LATTICES, UNIT CELLS --> CRYSTAL STRUCTURES



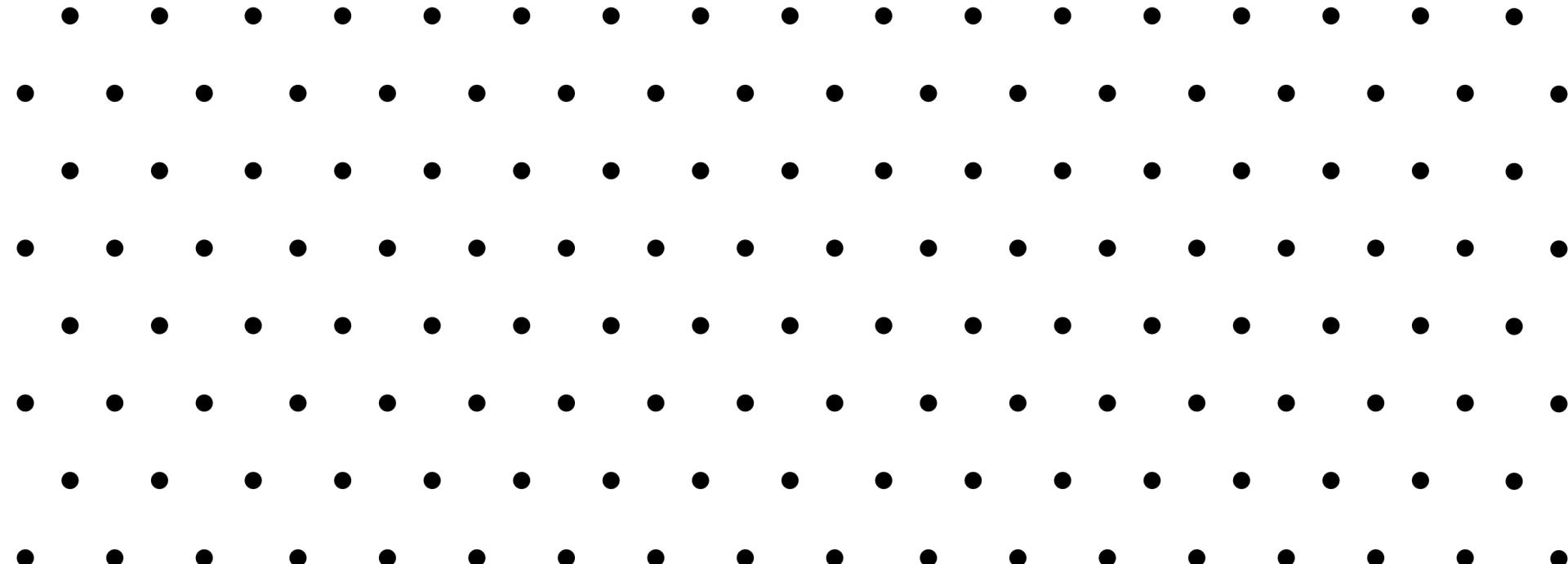
# M C. Escher





# LATTICE

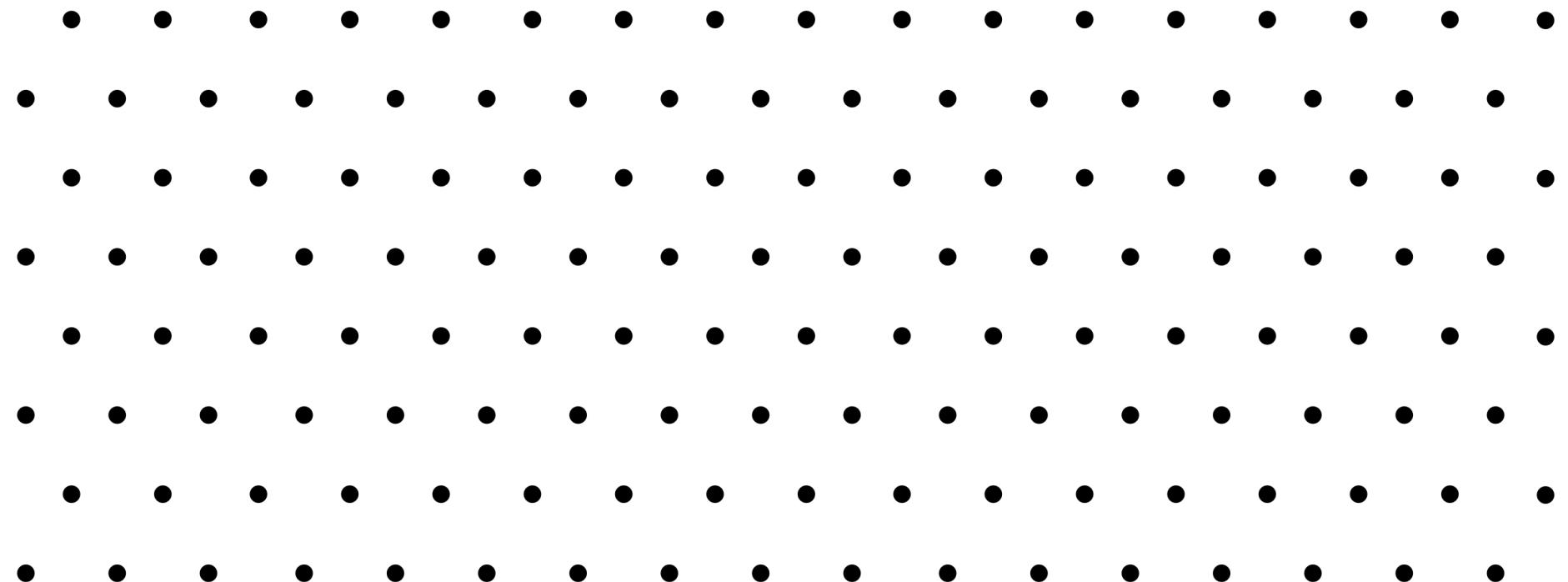
- a mathematical concept
- **Lattice:** infinite arrangement of points in space (3D)/ in the plane (2D)/ on a line (1D)  
in which all the points have same surroundings



# LATTICE

Geometry, group theory: an **infinite** set of points in the real coordinate space  $\mathbb{R}^n$

- addition or subtraction of two points in the lattice produces another lattice point
- lattice points are all separated by some minimum distance,
- every point in the space is within some maximum distance of a lattice point



# M.C. ESCHER Drawings

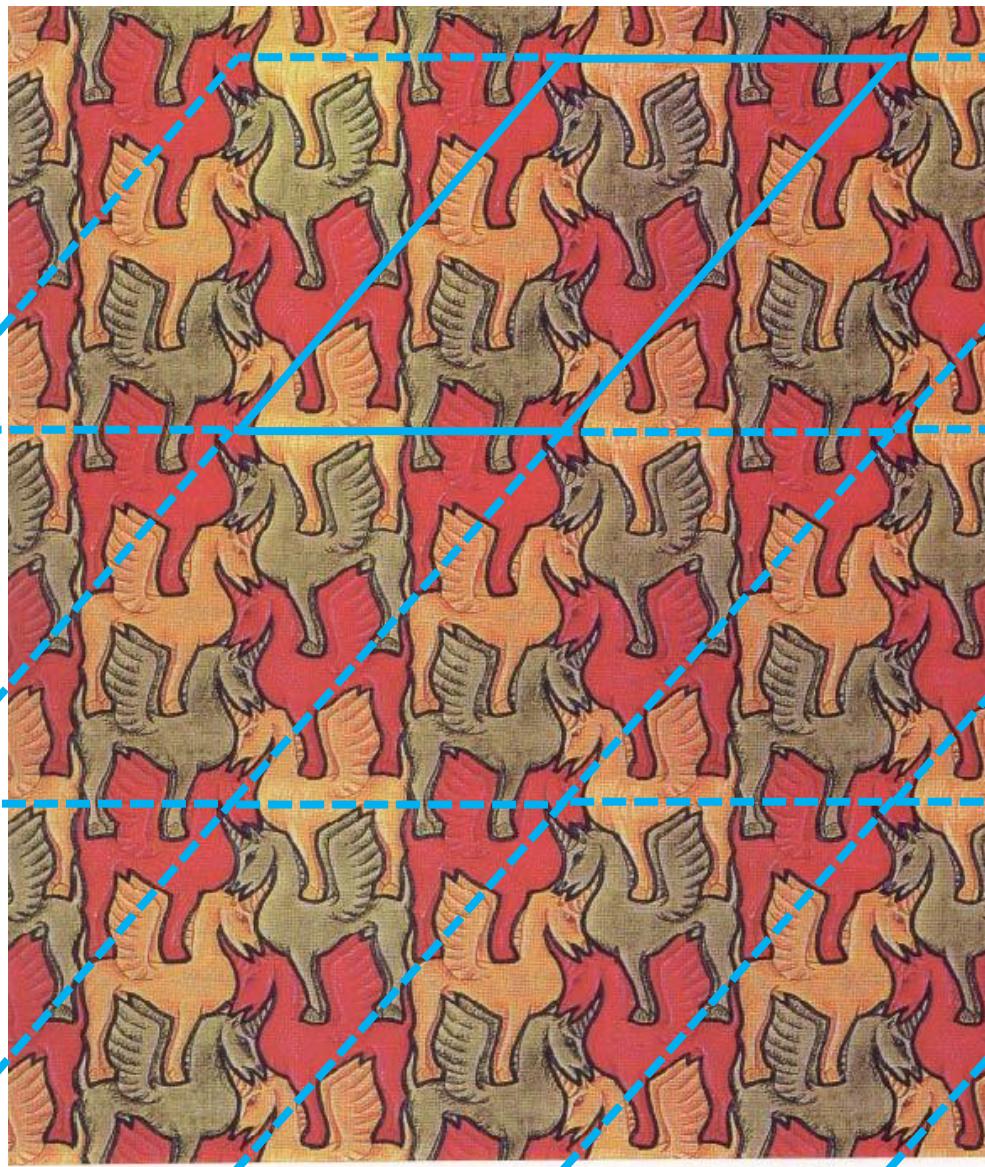


Figure 3. Escher Pattern #78 (*Unicorn*), reproduced with permission of Cordon Art.

# M.C. ESCHER Drawings

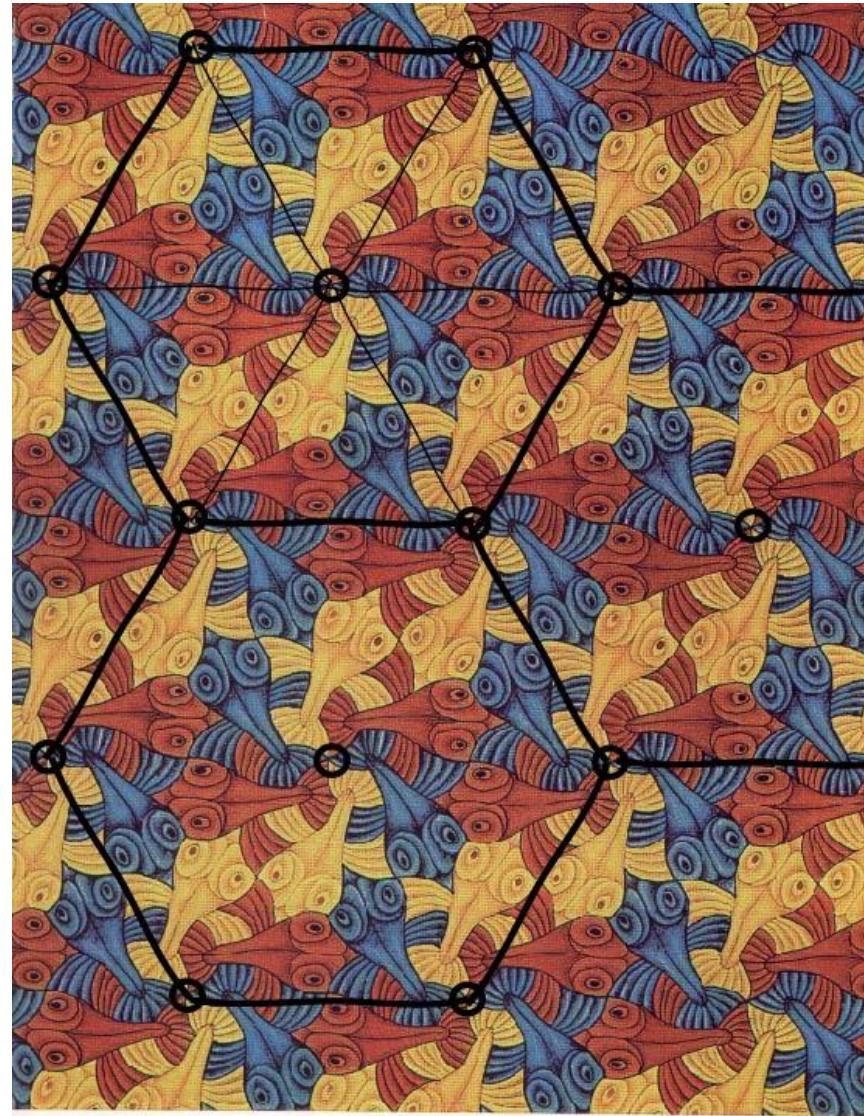


Figure 1. Escher Pattern #55 (*Fish*), reproduced with permission of Cordon Art.

# BRAVAIS LATTICES – PRIMITIVE LATTICE VECTORS

in 3D

3 lattice vectors

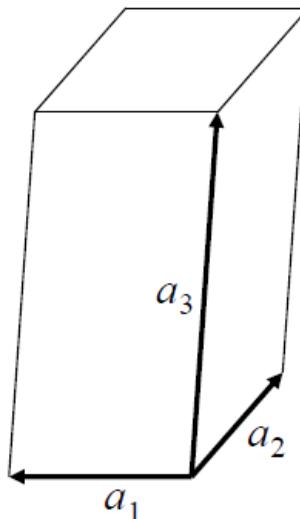
Every point of a Bravais lattice can be reached from another point on the lattice by a translation vector

$\mathbf{a}, \mathbf{b}, \mathbf{c}$

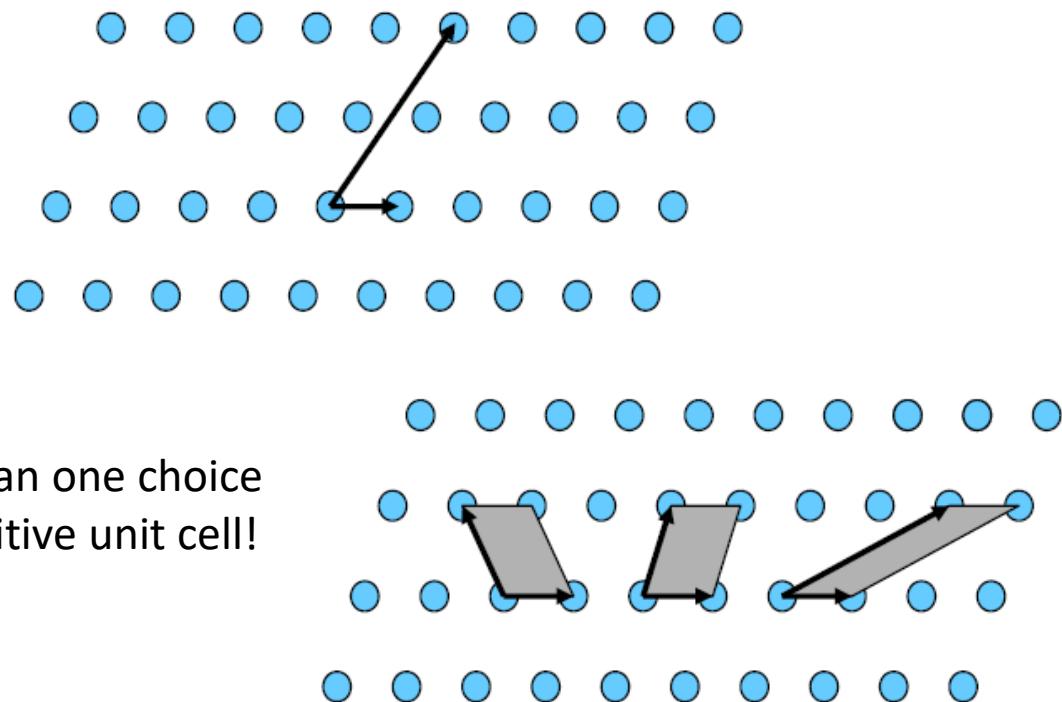
$$\vec{R} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c} \quad n_1, n_2, n_3 = \dots -2, -1, 0, 1, 2, 3 \dots$$

volume of unit cell:

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$$



more than one choice  
for primitive unit cell!



# BRAVAIS LATTICES

an infinite array of discrete points generated by a set of discrete translation operations described in 3D space by:

$$\vec{R} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

- 14 possible Bravais lattices in 3D space (only 5 in 2D)

P: Primitive (simple)  
I: body centered  
F: face centered  
C: centered on single face

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

Crystal family	Lattice system	Point group (Schönflies notation)	14 Bravais lattices					
			Primitive (P)	Base-centered (S)	Body-centered (I)	Face-centered (F)		
	Triclinic (a)	C <sub>i</sub>		aP				
	Monoclinic (m)	C <sub>2h</sub>		mP		mS		
	Orthorhombic (o)	D <sub>2h</sub>			oI		oF	
	Tetragonal (t)	D <sub>4h</sub>		tP			tl	
	Rhombohedral	D <sub>3d</sub>					hR	
Hexagonal (h)	Hexagonal	D <sub>6h</sub>		hP				
	Cubic (c)	O <sub>h</sub>		cP		cl		cF

# BRAVAIS LATTICES



Auguste Bravais

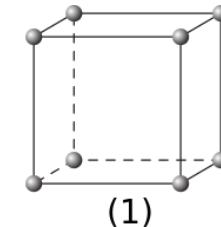
3D VIEW:

[The 14 Bravais lattices \(tugraz.at\)](http://tugraz.at)

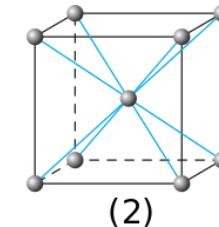
1.Cubic P

2.Cubic I

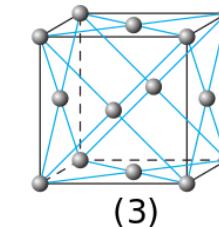
3.Cubic F



(1)



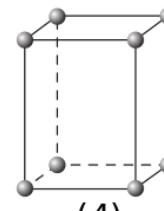
(2)



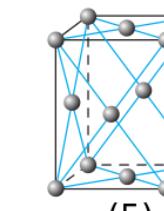
(3)

4.Tetragonal P

5.Tetragonal I



(4)



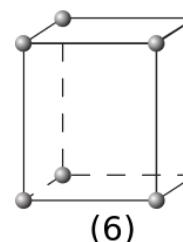
(5)

6.Orthorhombic P

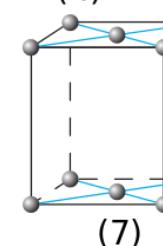
7.Orthorhombic C

8.Orthorhombic I

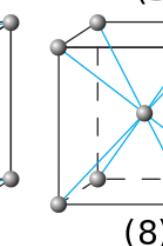
9.Orthorhombic F



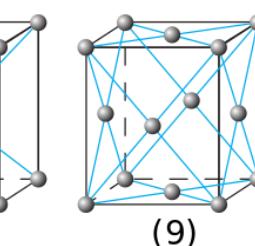
(6)



(7)



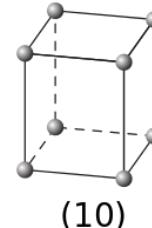
(8)



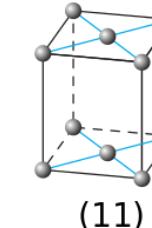
(9)

10.Monoclinic P

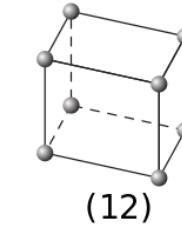
11.Monoclinic C



(10)



(11)

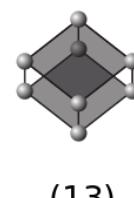


(12)

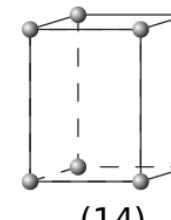
12.Triclinic

13.Rhomboedral

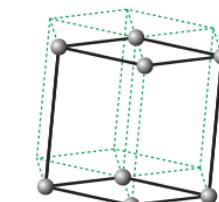
14.Hexagonal



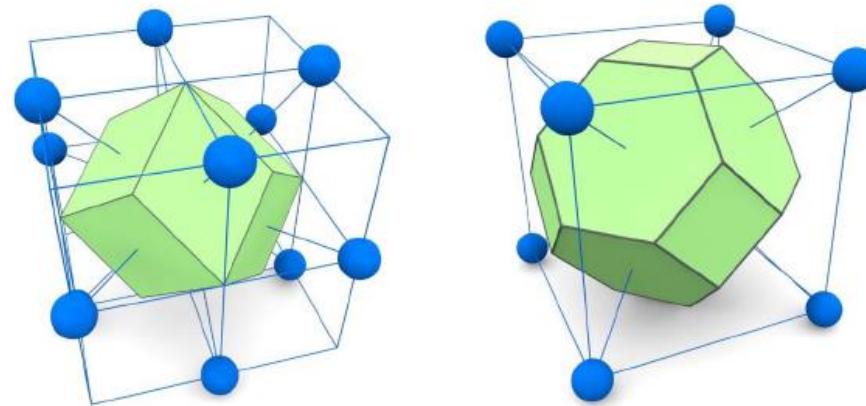
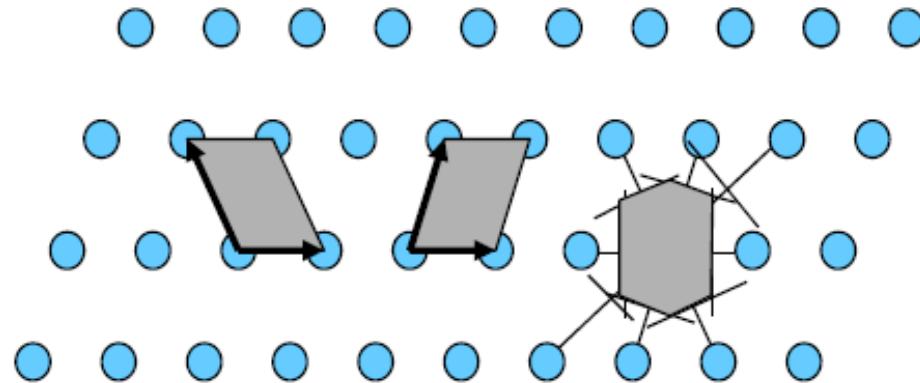
(13)



(14)



# UNIT CELL

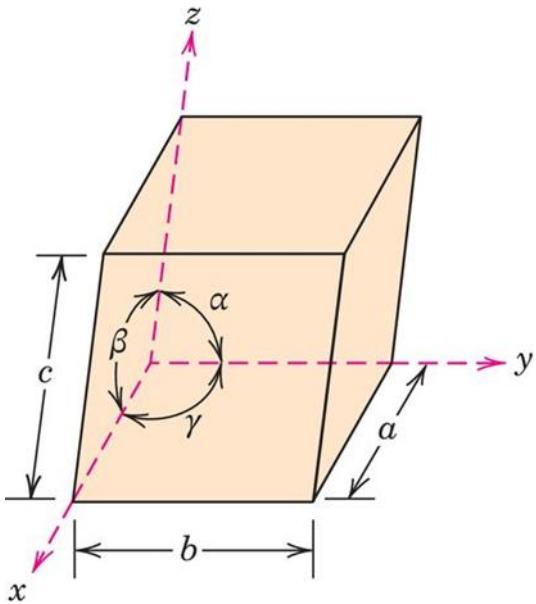


fcc

bcc

# CONVENTIONAL (CRYSTALLOGRAPHIC) UNIT CELL

- 7 crystal systems

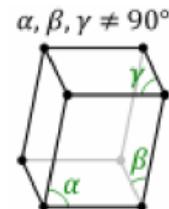


lattice parameters  
 $a, b, c$   
 $\alpha, \beta, \gamma$

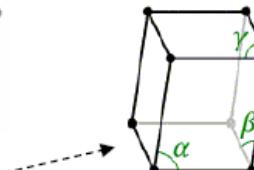
Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
<a href="#">VMSE: Crystal Systems and Unit Cells for Metals</a>			
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

# CRYSTAL SYSTEMS

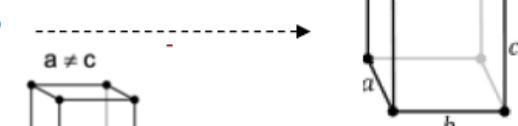
**triclinic:**  $a \neq b \neq c$  and  $\alpha \neq \beta \neq \gamma \neq 90^\circ$



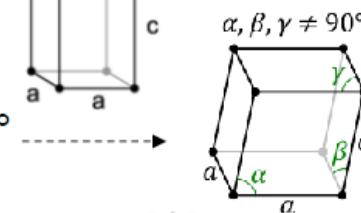
**monoclinic:**  $a \neq b \neq c$  and  $\alpha \neq 90^\circ$ ,  $\beta = \gamma = 90^\circ$



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



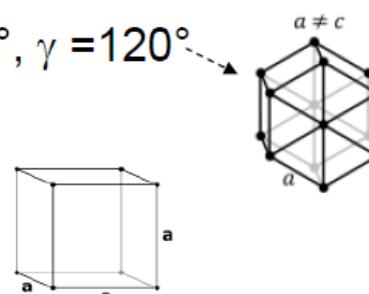
**tetragonal:**  $a = b \neq c$  and  $\alpha = \beta = \gamma = 90^\circ$



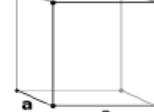
**rhombohedral:**  $a = b = c$  and  $\alpha \neq \beta \neq \gamma \neq 90^\circ$



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



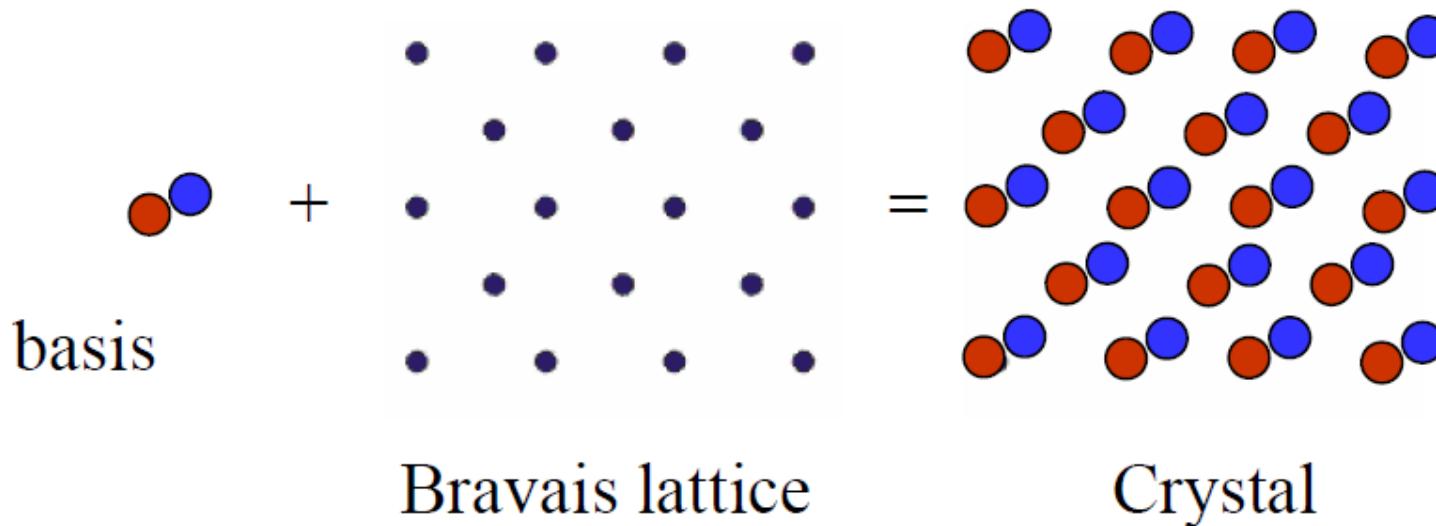
**cubic**  $a = b = c$  and  $\alpha = \beta = \gamma = 90^\circ$



$\alpha$  is the angle between b and c

(from P. Hadley, Solid State Physics, TUGraz)

# BRAVAIS LATTICES → CRYSTAL STRUCTURE



- **Bravais lattice ≠ Crystal structure !**
- basis may consist of atoms, molecules, or polymer strings
- the lattice provides the locations of the basis



# CRYSTAL = LATTICE + MOTIF (BASIS)

## CRYSTAL = LATTICE + MOTIF

### YOUTUBE VIDEO

Unit 1.9 of the course «The Fascination of Crystal and Symmetry»  
by F. Hoffmann, Univ. Hamburg

[Unit 1.9 - Crystal = Lattice + Motif - YouTube](#)



L3.3

# CRYSTAL STRUCTURES, PACKING OF ATOMS

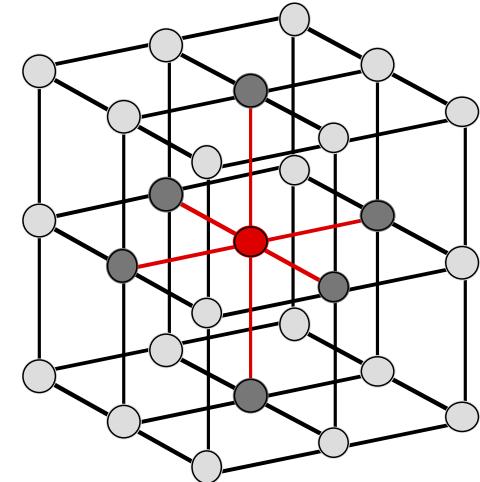
# METALLIC CRYSTAL STRUCTURES: ATOMIC PACKING

- **Dense atomic packing** for crystal structures of metals
- Reasons for dense packing:
  - Bonds between metal atoms are nondirectional
  - Nearest neighbor distances tend to be small in order to lower bond energy
  - High degree of shielding (of ion cores) provided by free electron cloud
- Crystal structures for metals simpler than structures for ceramics and polymers

# DEFINITIONS

coordination number

CN = number of nearest-neighbor  
or touching atoms



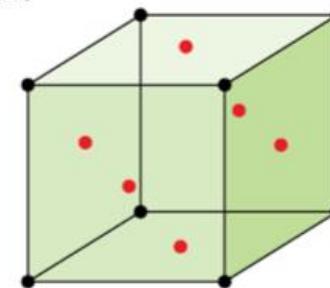
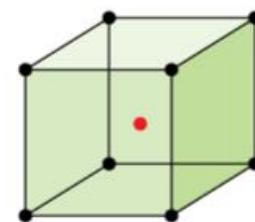
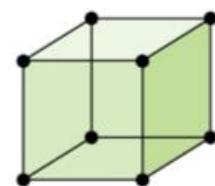
atomic packing factor

$$\text{APF} = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

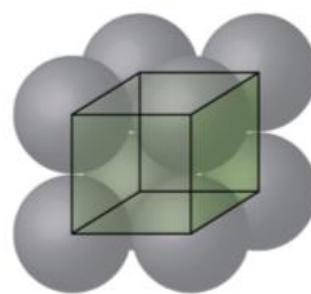
\*assume hard spheres

# CUBIC STRUCTURES

Lattice point locations

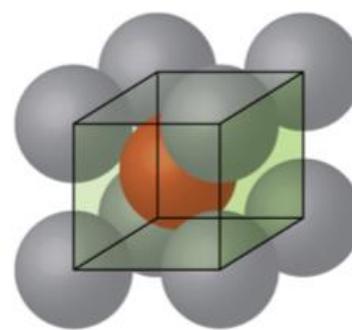


Cubic unit cells



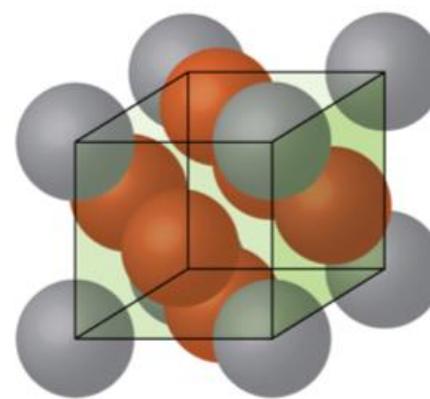
Primitive cubic

SC



Body-centered cubic

bcc



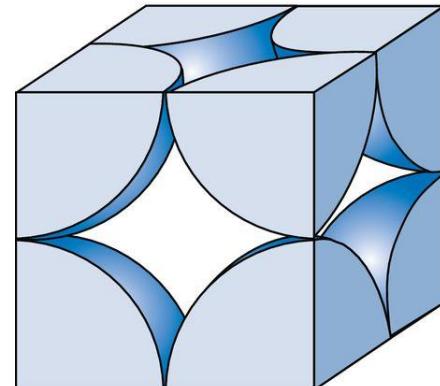
Face-centered cubic

fcc

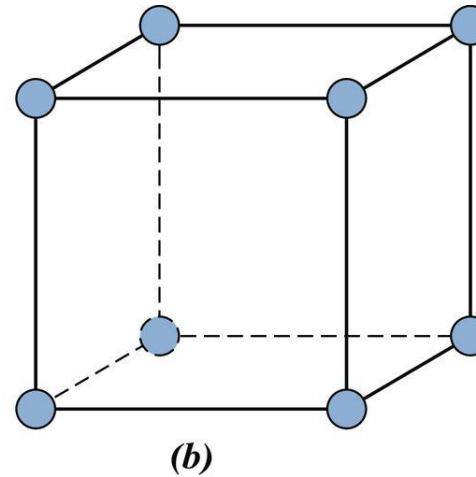
# SIMPLE CUBIC (CUBIC P)

SC

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

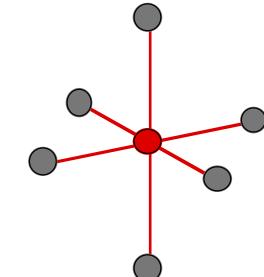
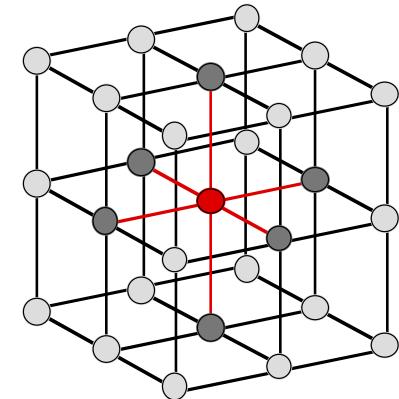


(a)

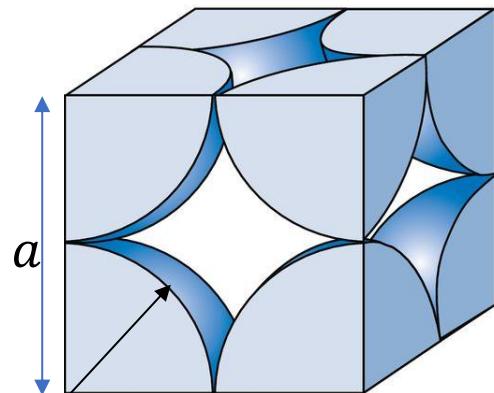


(b)

- 1 atom/unit cell
- CN: coordination number = 6
- APF = 0.52
- Close-packed directions: cube edges
- Rare in metals due to low packing density  
(only Po has this structure)



# APF – SIMPLE CUBIC



$$R = \frac{1}{2}a$$

[3D viewer - VMSE BCC](#)

[JSmol – simple cubic \(tugraz.at\)](#)

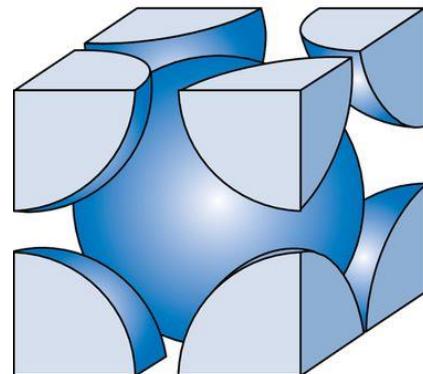
n. atoms in unit cell

volume atom

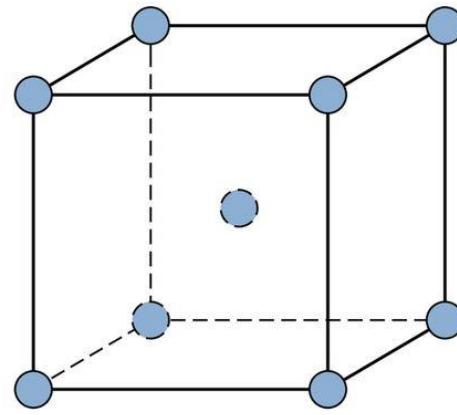
$$\text{APF} = \frac{1 \cdot \frac{4}{3}\pi R^3}{a^3} = \frac{1 \cdot \frac{4}{3}\pi \left(\frac{1}{2}a\right)^3}{a^3} = 0.52$$

volume unit cell

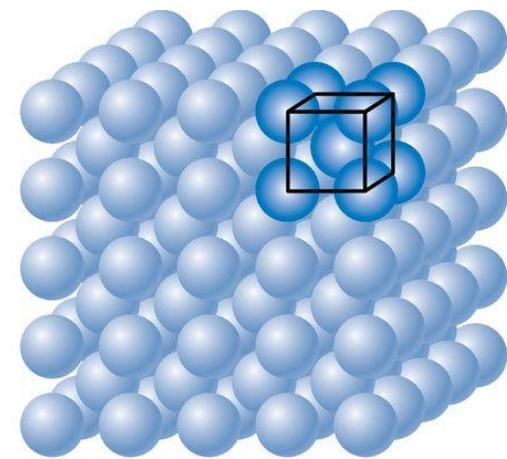
# BODY CENTERED CUBIC (CUBIC I)

**BCC**

(a)



(b)

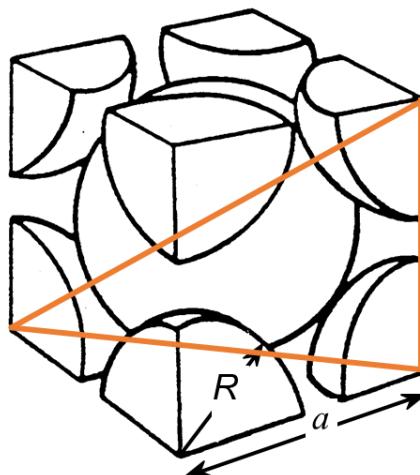
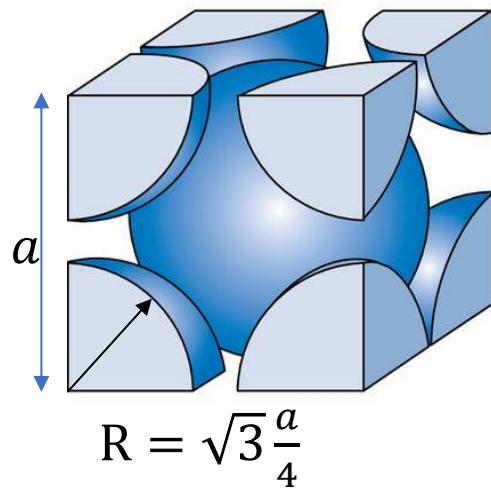


(c)

- 2 atoms/unit cell
- CN: = 8
- APF = 0.68
- Cr, W, Fe, Ta, Mo

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

[3D viewer - VMSE FCC](#)[JS Mol - Body centered cubic \(tugraz.at\)](#)



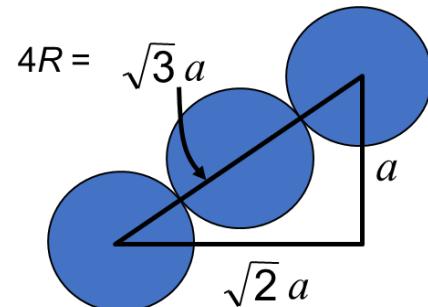
# APF – BCC

n. atoms in unit cell

volume atom

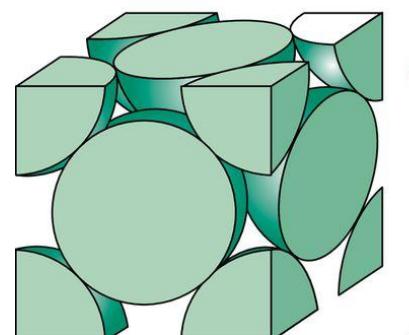
$$\text{APF} = \frac{2 \cdot \frac{4}{3} \pi R^3}{a^3} = \frac{2 \cdot \frac{4}{3} \pi \left(\frac{\sqrt{3}a}{4}\right)^3}{a^3} = 0.68$$

volume unit cell

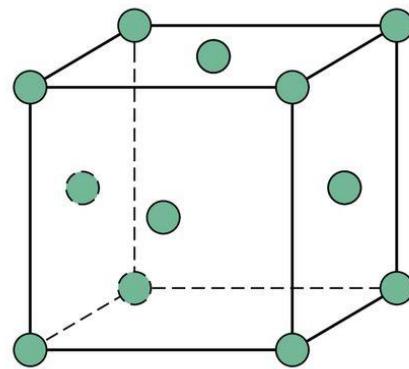


# FACE CENTERED CUBIC (CUBIC F)

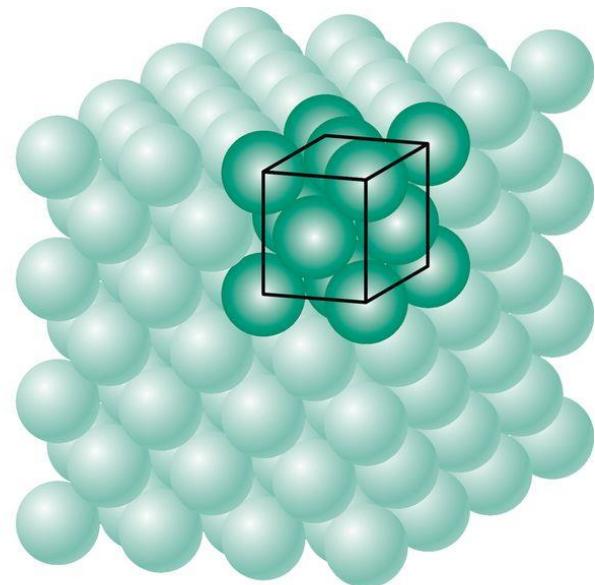
FCC

[3D viewer - VMSE FCC](#)[Jsmol - fcc \(tugraz.at\)](#)

(a)



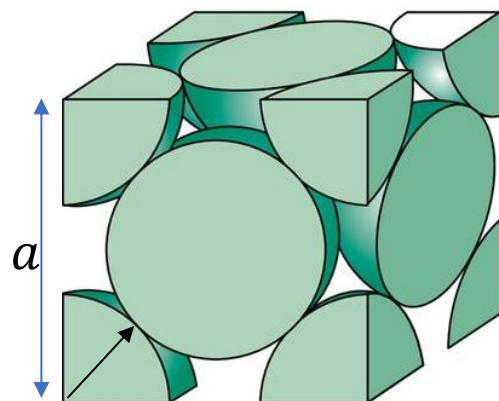
(b)



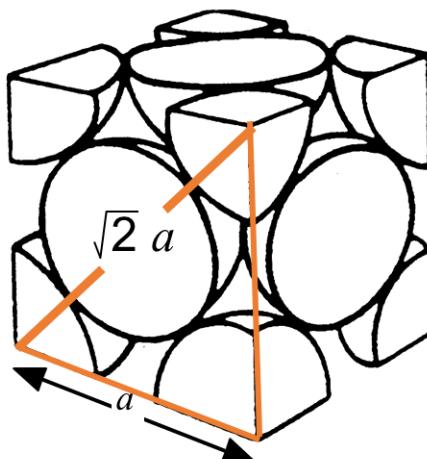
(c)

- 4 atoms/unit cell
- CN: = 12
- APF = 0.74      max. possible packing of spheres!
- Al, Ag, Ni, Au, Pb, Pt, Cu,...

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



$$R = \sqrt{2} \frac{a}{4}$$



$$4R = \sqrt{2}a$$

# APF – FCC

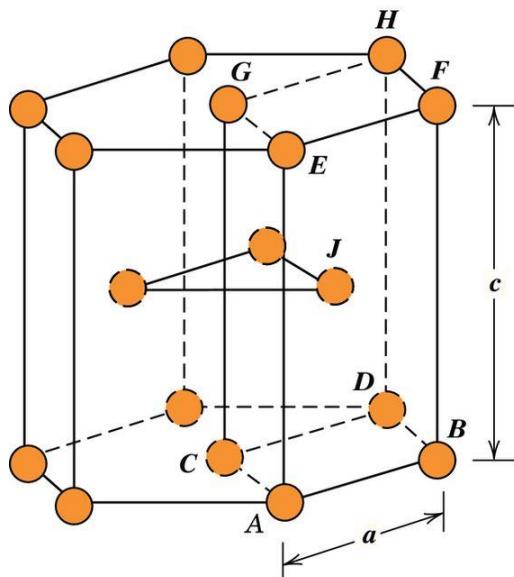
n. atoms in unit cell

volume atom

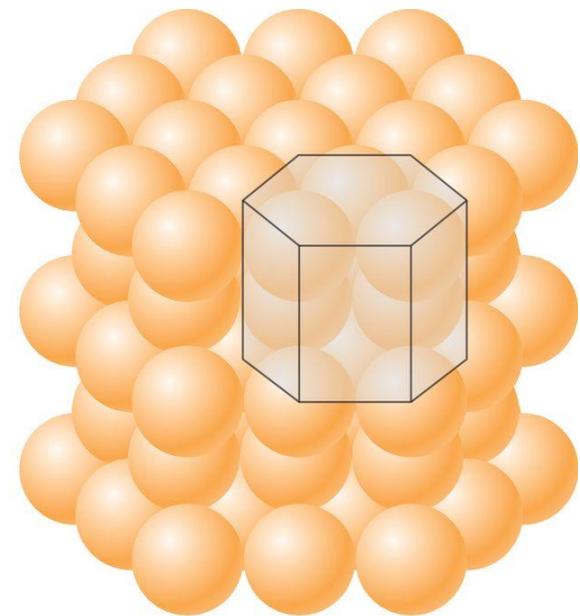
$$\text{APF} = \frac{4 \cdot \frac{4}{3}\pi R^3}{a^3} = \frac{4 \cdot \frac{4}{3}\pi \left(\sqrt{2}\frac{a}{4}\right)^3}{a^3} = 0.74$$

volume unit cell

## HCP

3D viewer - VMSE HCPJSmol - HCP (tugraz.at)

- 6 atoms/unit cell
- CN: = 12 same as FCC!
- APF = 0.74 max. possible packing of spheres!
- ideal c/a=1.633
- Cd, Mg, Ti, Zn...



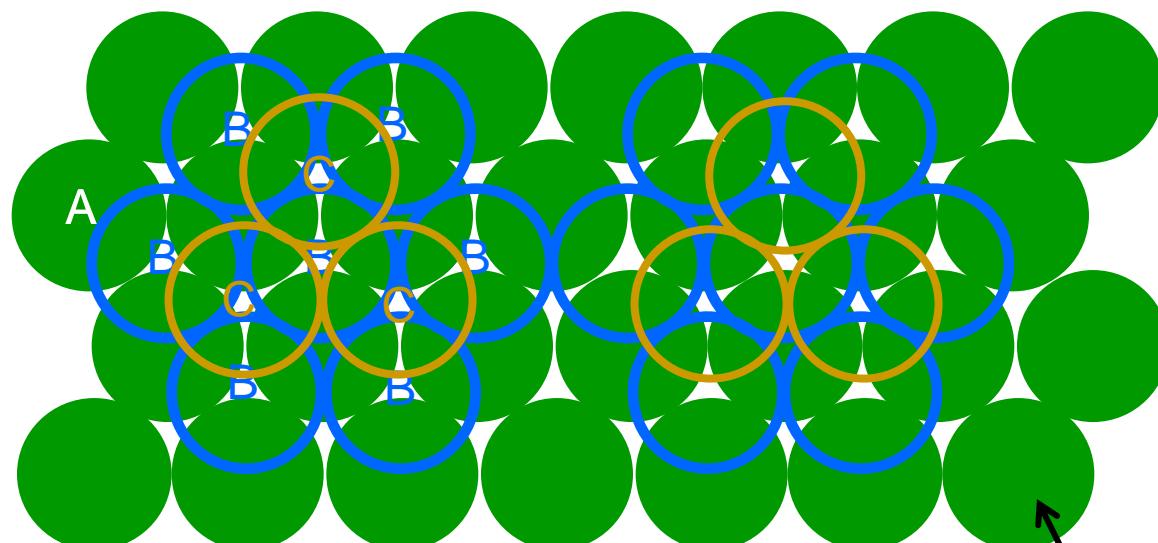
$$3 + 2 \times \frac{1}{2} + 12 \times \frac{1}{6} = 6$$

# CLOSE PACKING - FCC PLANE STACKING SEQUENCE

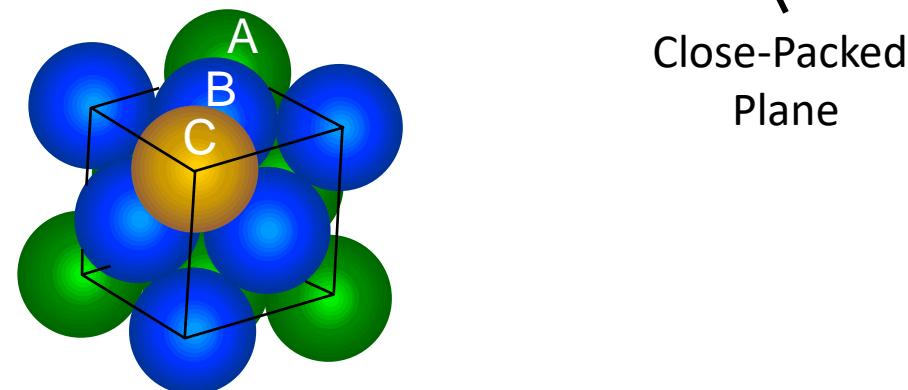
- ABCABC... Stacking Sequence—Close-Packed Planes of Atoms

2D Projection

A sites  
B sites  
C sites



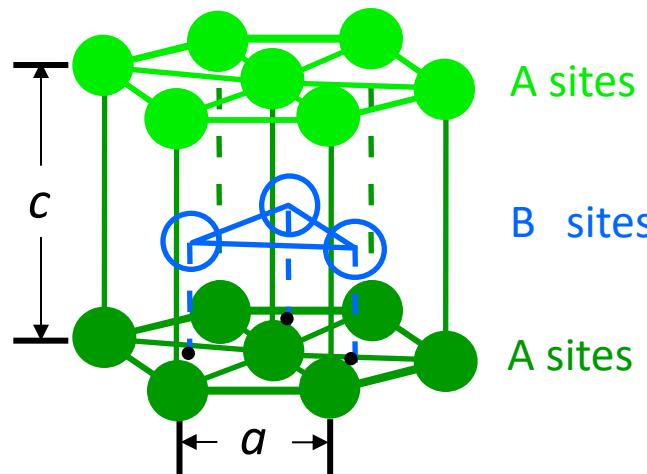
- Stacking Sequence referenced to an FCC Unit Cell



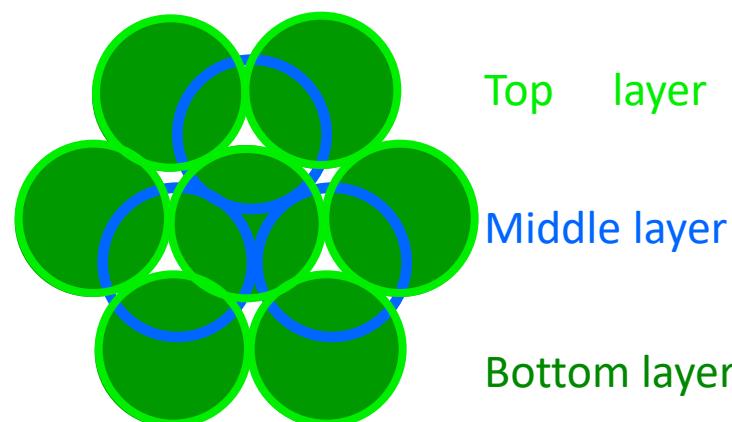
# CLOSE PACKING - HCP PLANE STACKING SEQUENCE

- ABAB... Stacking Sequence—Close-Packed Planes of Atoms

- 3D Projection



- 2D Projection



Hexagonal Close Packing

[3D viewer – VMSE Close packed structures](#)



# COMMON CRYSTAL STRUCTURES

[Course outline Solid State Physics \(tugraz.at\)](#)

collection of crystal structures (by Prof. P. Hadley, Inst Solid State physics, TUGraz, Austria)

[Jsmol - Diamond \(tugraz.at\)](#)

[Jsmol - NaCl \(tugraz.at\)](#)

[Jsmol - Graphite \(tugraz.at\)](#)

[Jsmol - Zincblend \(ZnS\) \(tugraz.at\)](#)

[Jsmol - Silicon \(tugraz.at\)](#)

[Jsmol – Perovskite \(CaTiO<sub>3</sub>\) \(tugraz.at\)](#)

[JSmol – YBCO \(high temp superconductor\) \(tugraz.at\)](#)

[Jsmol – ZIF8 \(Zeolite\) \(tugraz.at\)](#)



L3.4

# DENSITY, POLYMORPHISM

# THEORETICAL DENSITY FOR METALS, $\rho$

$$\rho = \frac{\text{Mass in unit cell}}{\text{Volume of unit cell}}$$

$$\rho = \frac{nA}{V_C N_A}$$

$n$  = number of atoms/unit cell

$A$  = atomic weight

$V_C$  = volume of unit cell

$N_A$  = Avogadro's number =  $6.02214076 \times 10^{23}$  atoms/mol

## PROBLEM (for next lesson)

- Calculate theoretical  $\rho$  of:

**Cu, Cr** (look for atomic radius  $R$ , crystal structure, atomic weight  $A$ )

- Compare with actual  $\rho$  (literature)

# DENSITIES COMPARISON

$$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$$

Based on data in Table B1, Callister

Why?

Metals

- close-packing (metallic bonding)
- often large atomic masses

Ceramics

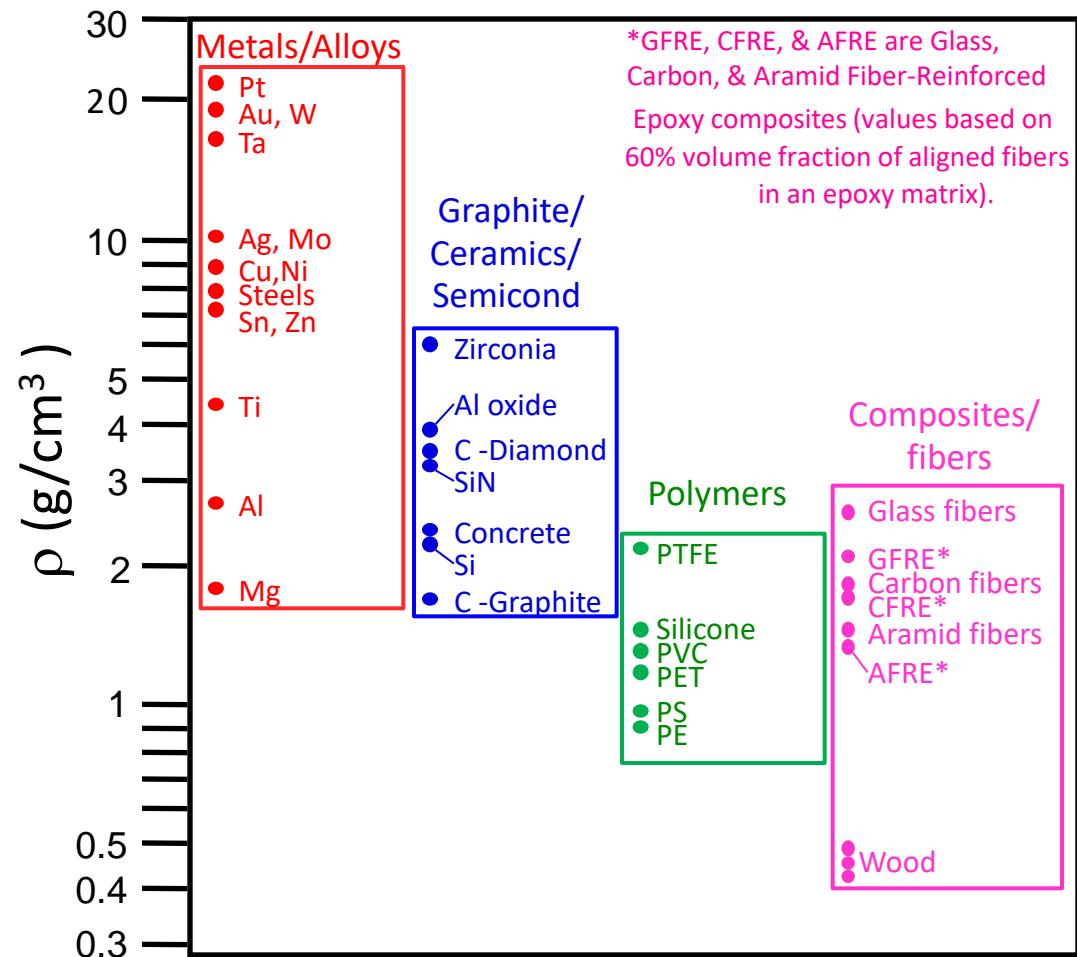
- often lighter elements

Polymers

- low packing density  
(often amorphous)
- lighter elements (C,H,O)

Composites

- moderate to low densities

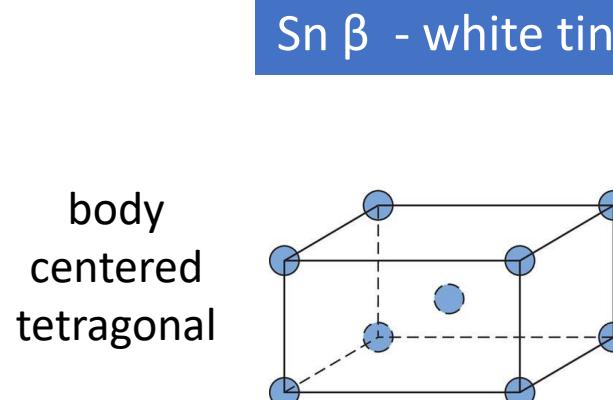




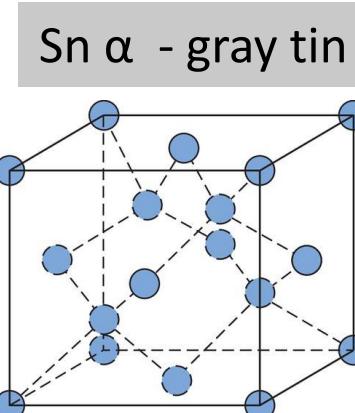
# POLYMORPHISM, ALLOTROPY

- crystalline materials can have more than one possible crystal structure : POLYMORPHISM (different conditions during formation)
- polymorphism in elements: ALLOTROPY

# POLYMORPHISM, ALLOTROPY – EXAMPLE: Sn



13.2°C  
Cooling

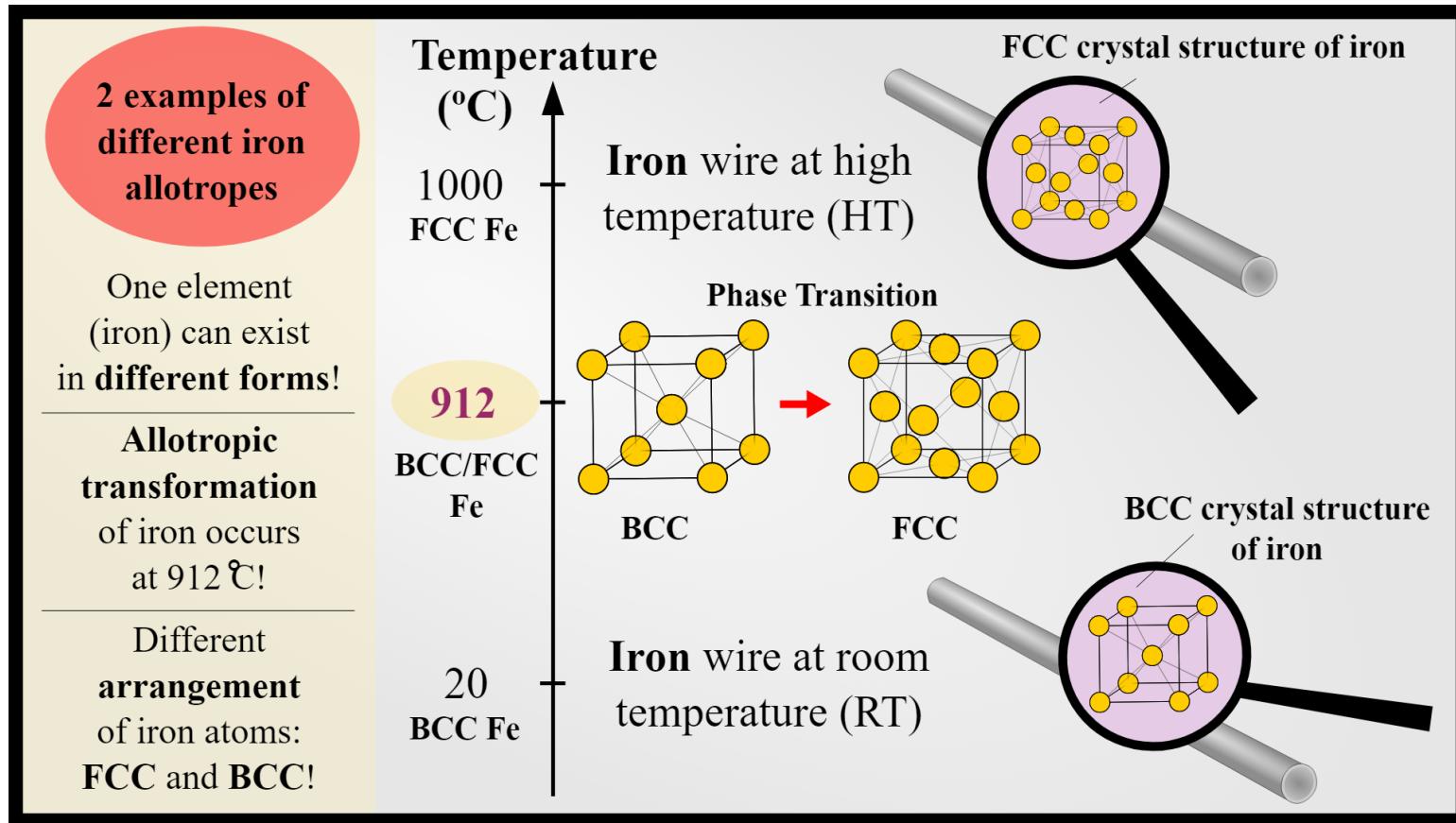


FCC – 2 atoms basis  
(diamond-like)



Photograph courtesy of Professor Bill Plumbridge, Department of Materials Engineering, The Open University, Milton Keynes, England.

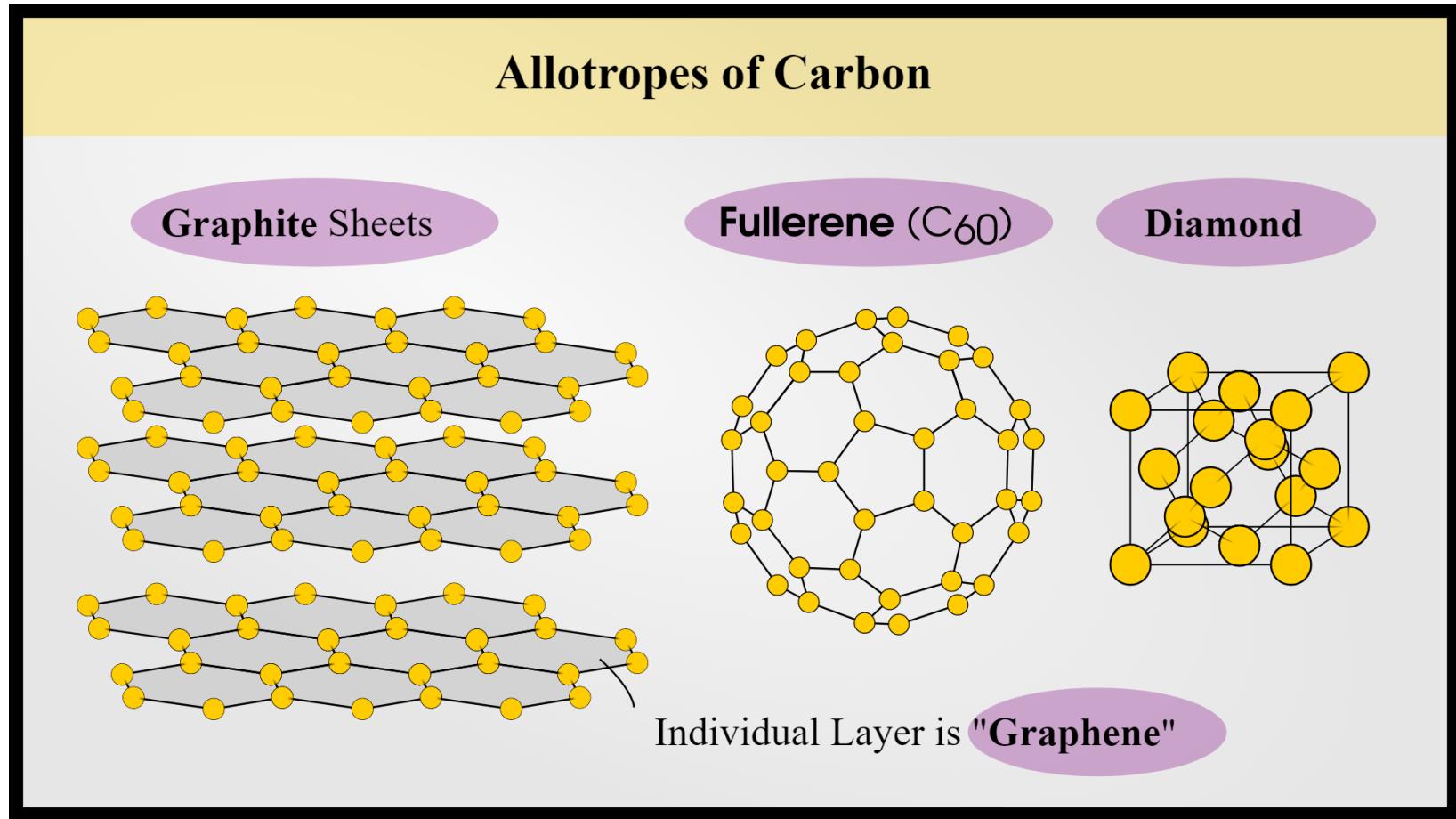
# POLYMORPHISM, ALLOTROPY – EXAMPLE: Fe



Source: <https://msestudent.com/>

more on Fe phases in L5!

# POLYMORPHISM, ALLOTROPY – EXAMPLE: C



Source: <https://msestudent.com/>



L3.5

# POINTS, DIRECTIONS, CRYSTALLOGRAPHIC PLANES

# POINT COORDINATES

A **point coordinate** is a lattice position in a unit cell

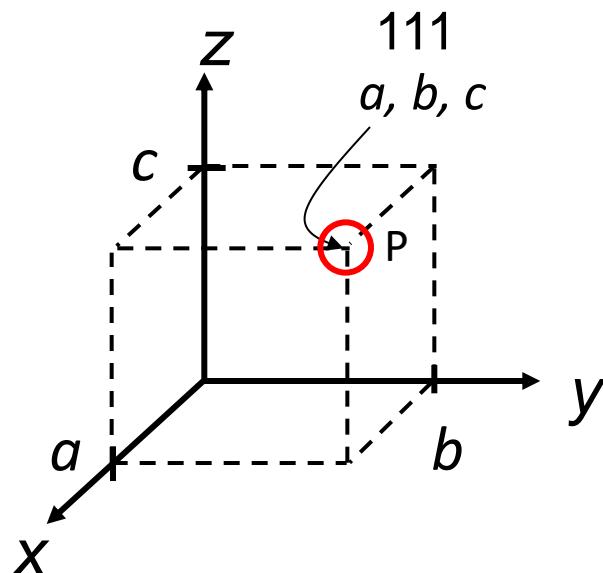
Determined as fractional multiples of  $a$ ,  $b$ , and  $c$  unit cell edge lengths

Example: Unit cell upper corner

1. Lattice position is

$$a, b, c$$

2. Divide by unit cell edge lengths ( $a$ ,  $b$ , and  $c$ )



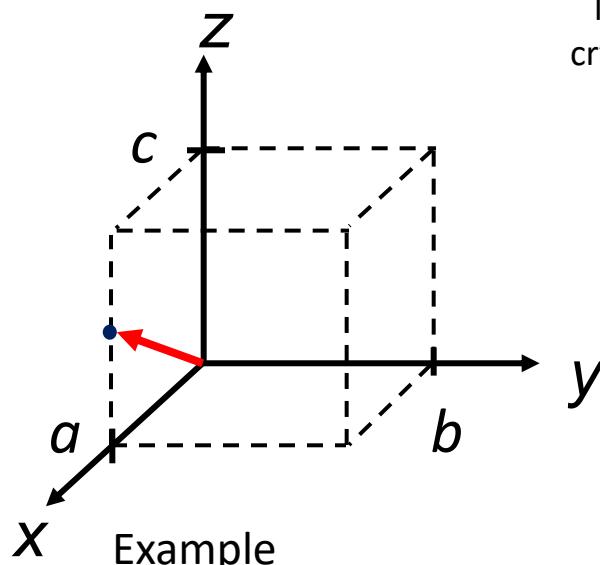
$$\frac{a}{a} \frac{b}{b} \frac{c}{c} = 111$$

3. Point coordinates for unit cell corner are **111**

# MILLER INDICES: CRYSTAL DIRECTIONS

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

lattice vectors of the  
crystallographic unit cell



Vector:

2 points  $(x_1, y_1, z_1); (x_2, y_2, z_2)$

$$\frac{x_2 - x_1}{a} \quad \frac{y_2 - y_1}{b} \quad \frac{z_2 - z_1}{c}$$

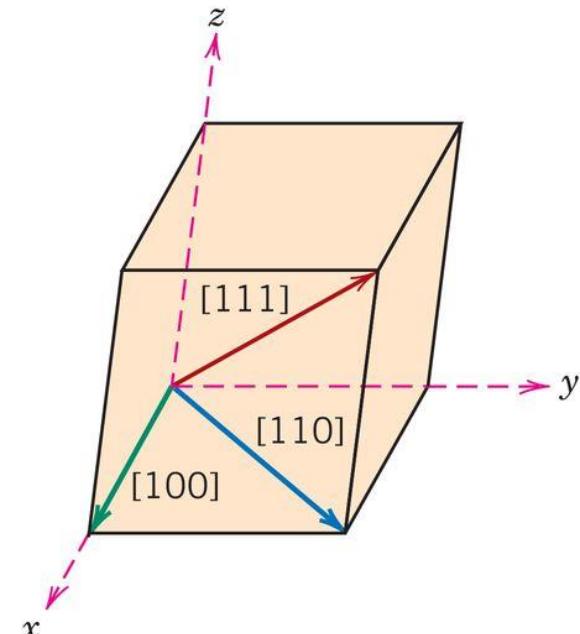
u      v      w

[u v w]

$$\frac{a-0}{a} \quad \frac{0-0}{b} \quad \frac{c/2-0}{c}$$

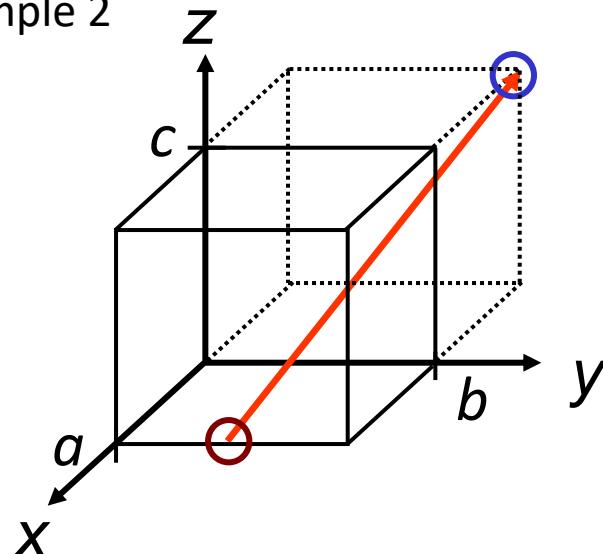
$$1 \ 0 \ \frac{1}{2} \rightarrow [2 \ 0 \ 1]$$

integer values



# MILLER INDICES: CRYSTAL DIRECTIONS

Example 2

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

$$\begin{matrix} -2 & \frac{1}{2} & 1 \\ \downarrow & & \\ -4 & 1 & 2 \end{matrix}$$

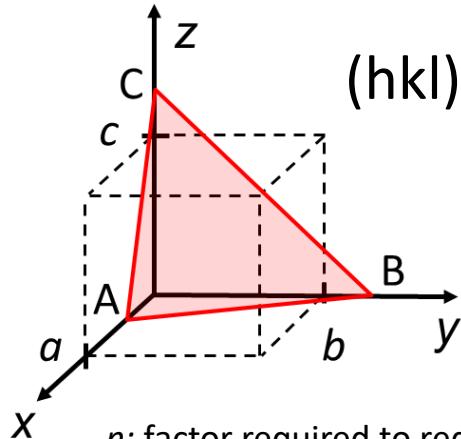
$$[\bar{4} \ 1 \ 2]$$

**Family of directions** – all directions that are crystallographically equivalent (have the same atomic spacing) – indicated by indices in angle brackets

Ex:  $\langle 100 \rangle = [100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]$

# MILLER INDICES: CRYSTAL PLANES

plane (hkl) intercepts axes at A,B,C



summary

$$h = n \frac{a}{A}$$

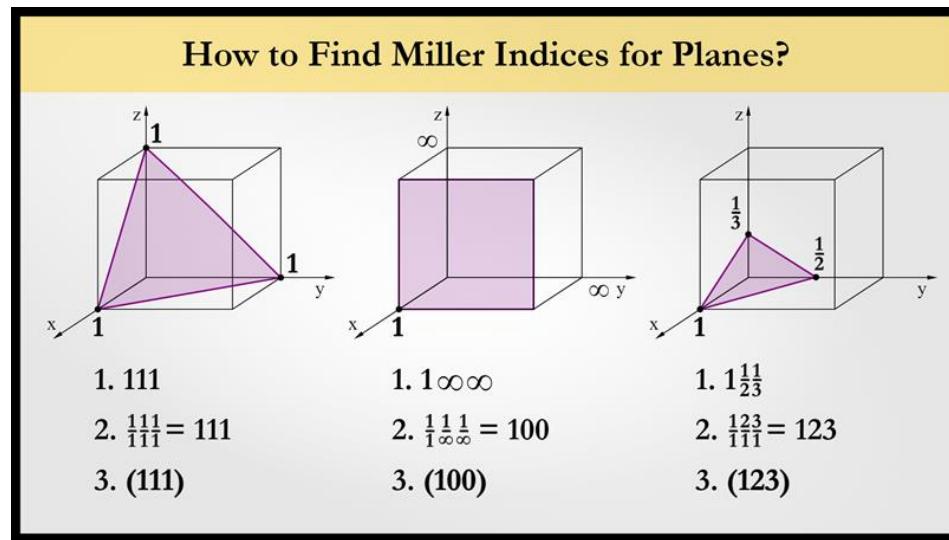
$$k = n \frac{b}{B}$$

$$l = n \frac{c}{C}$$

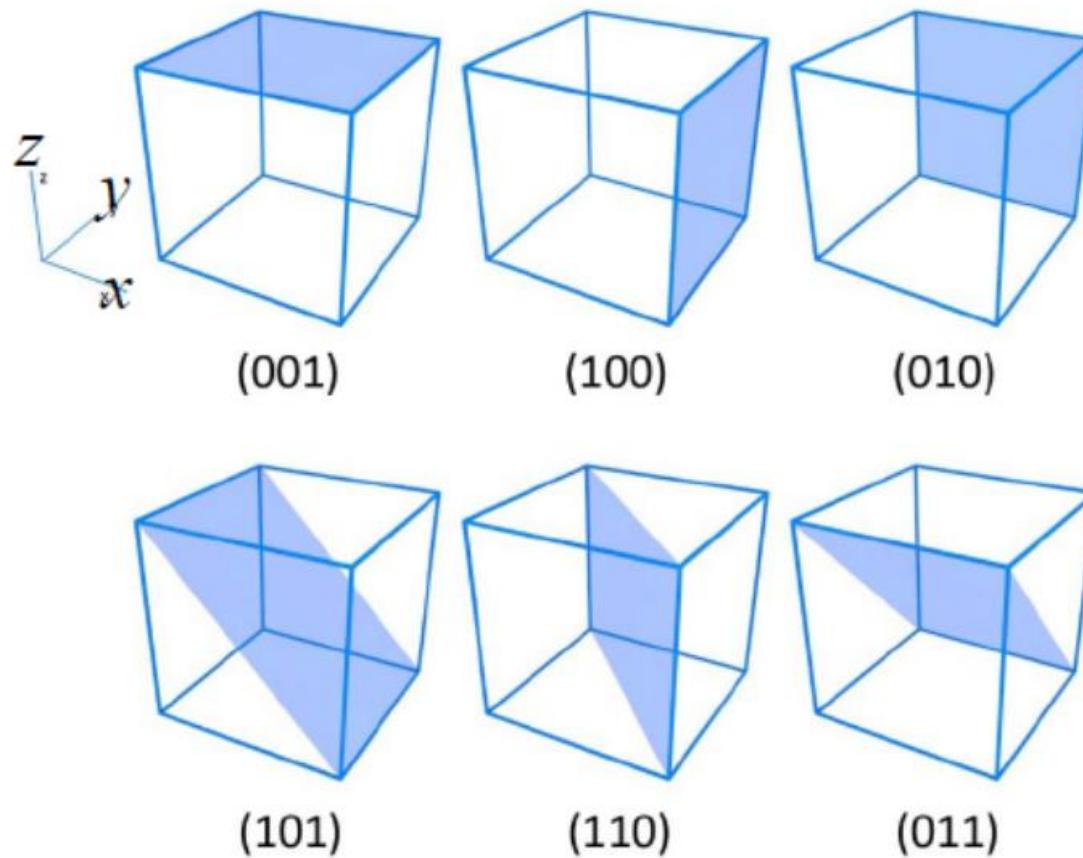
n: factor required to reduce h, k, and l to integers

step by step procedure

1. If plane passes through origin, establish a new origin in another unit cell
2. Read off values of intercepts of plane (A, B, C) with x, y, z axes in terms of a, b, c
3. Take **reciprocals of intercepts**
4. Reduce to smallest integer values
5. Enclose resulting **Miller Indices** in parentheses (**hkl**)



# CRYSTAL PLANES

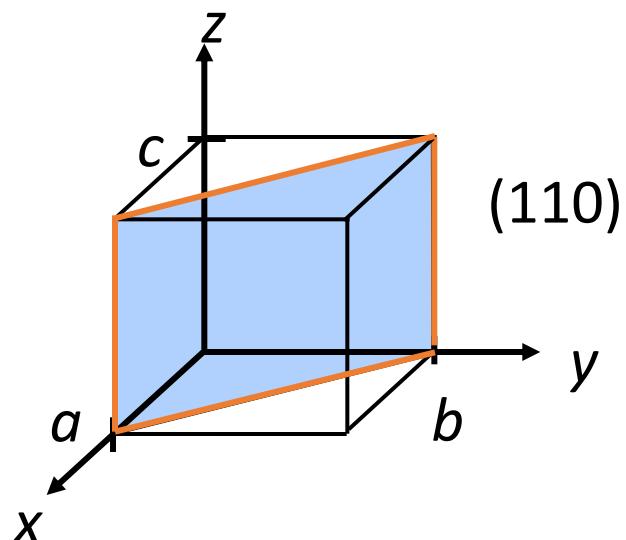


# CRYSTALLOGRAPHIC PLANES

## Example Problem I

$x \quad y \quad z$

1. Relocate origin – not needed
2. Intercepts  $a \quad b \quad \infty$
3. Reciprocals  $1/a \quad 1/b \quad 1/\infty$
4. Reduction  $1 \quad 1 \quad 0$
5. Miller Indices  $(110)$

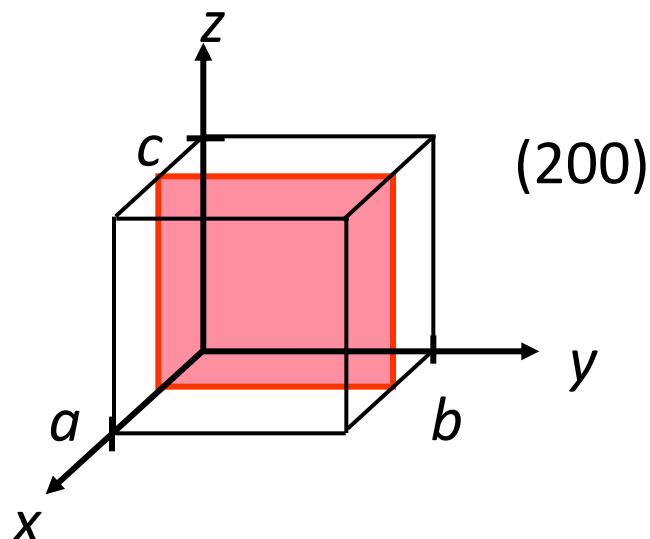


# CRYSTALLOGRAPHIC PLANES

## Example Problem II

x      y      z

1. Relocate origin – not needed
2. Intercepts             $a/2$      $\infty$      $\infty$
3. Reciprocals            $2/a$      $1/\infty$      $1/\infty$
4. Reduction            2        0        0
5. Miller Indices        (200)

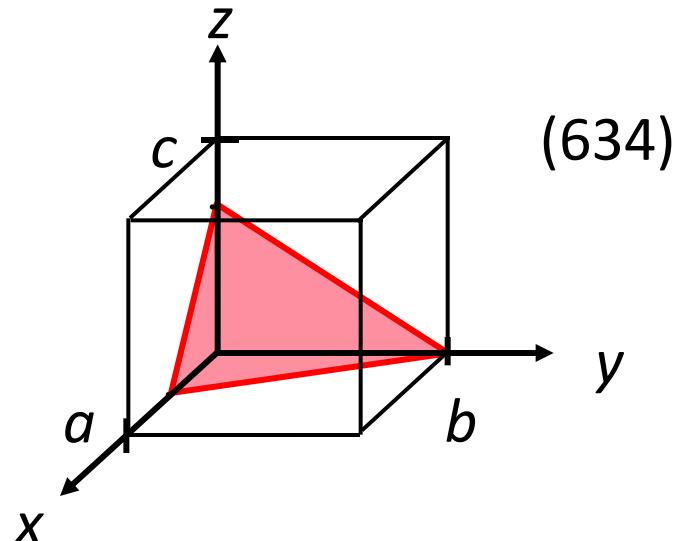


# CRYSTALLOGRAPHIC PLANES

## Example Problem III

	x	y	z
--	---	---	---

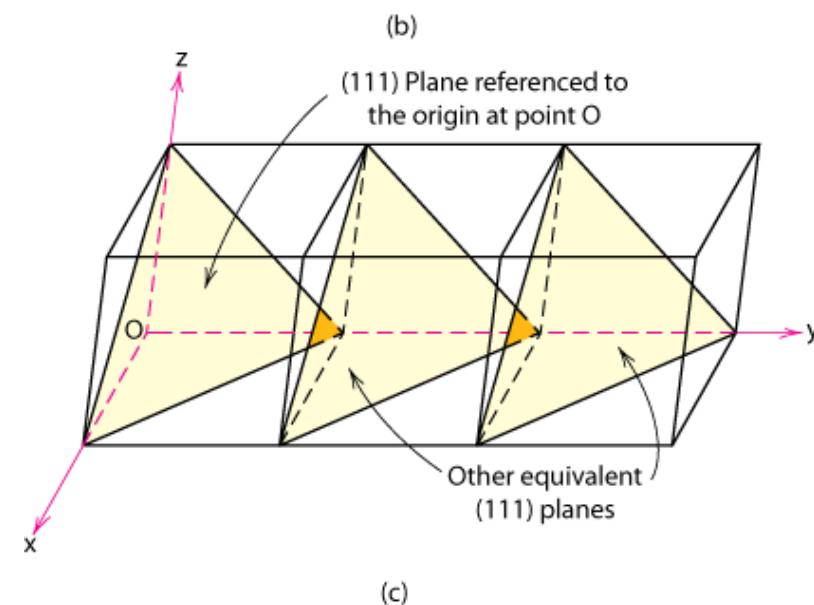
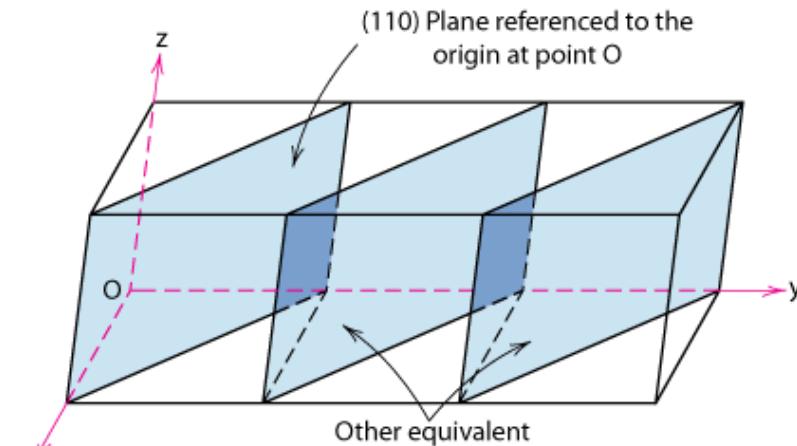
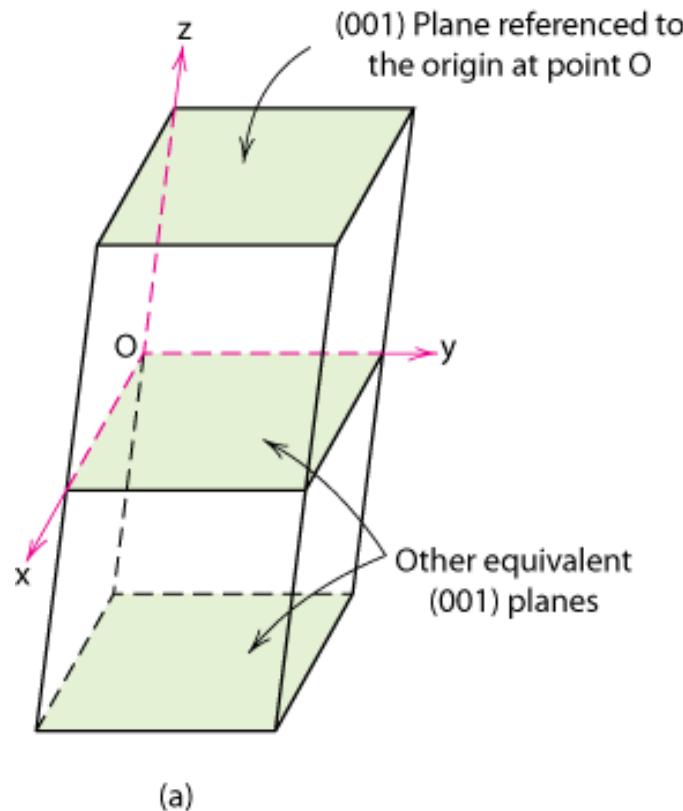
1. Relocate origin – not needed
2. Intercepts               $a/2$       b       $3c/4$
3. Reciprocals               $2/a$        $1/b$        $4/3c$
4. Reduction              6      3      4
5. Miller Indices      (634)



**Family of planes** – all planes that are crystallographically equivalent (have the same atomic packing) – indicated by indices in braces

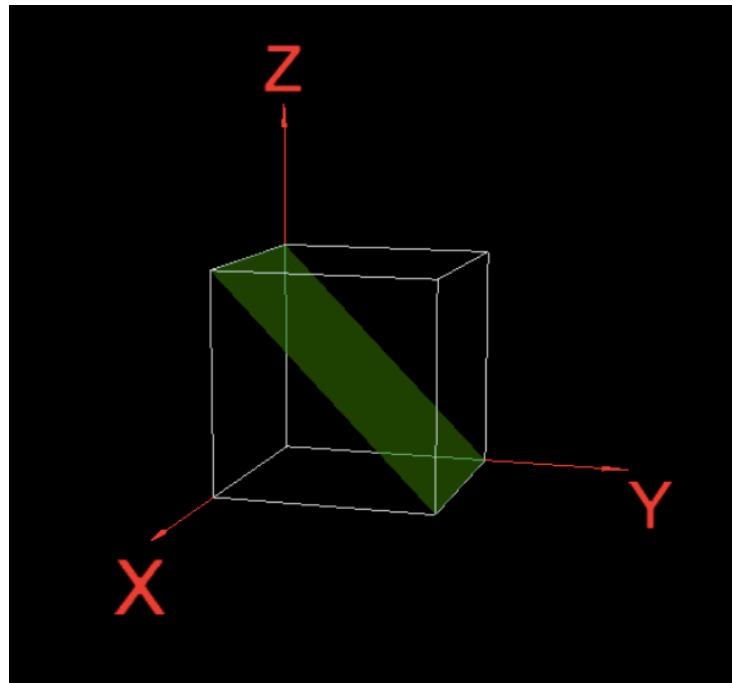
Ex:  $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

# COMMON CRYSTALLOGRAPHIC PLANES



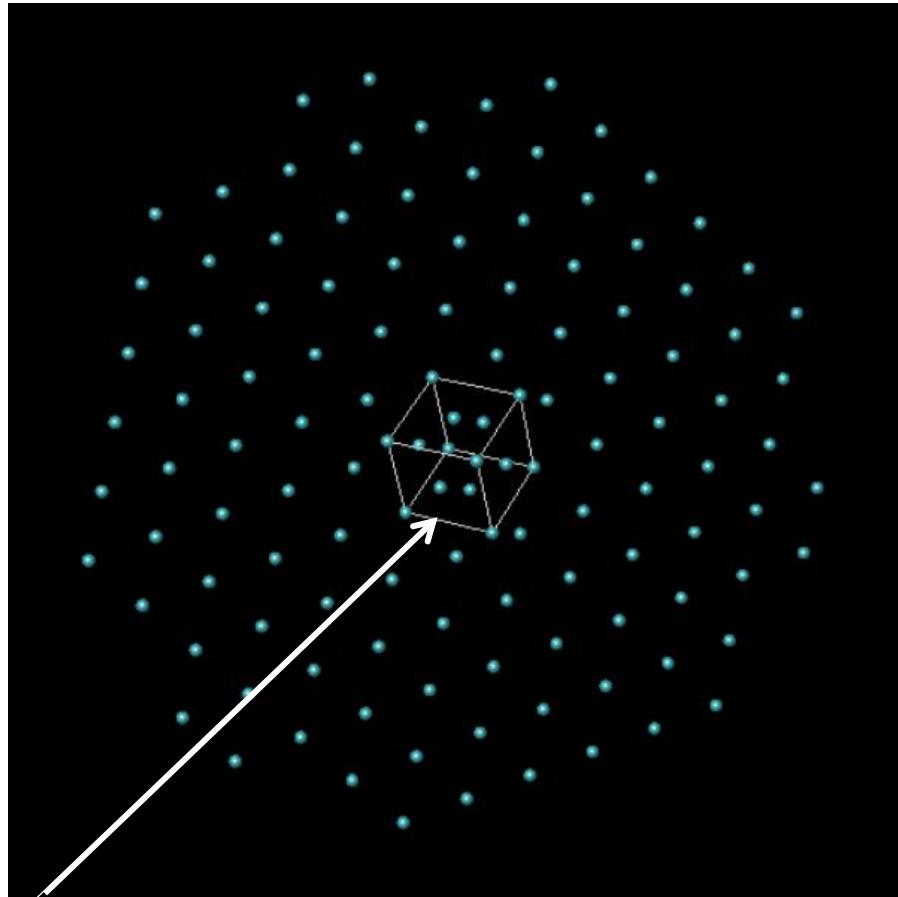
Adapted from Fig. 3.11,  
Callister & Rethwisch 9e.

# VMSE SCREENSHOT – CRYSTALLOGRAPHIC PLANES



3D view VMSE crystal planes

# PLANAR ATOMIC ARRANGEMENTS



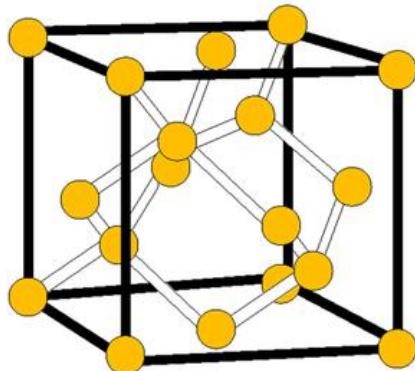
FCC Unit Cell

[3D viewer VMSE](#)



# Why crystal planes are important?

# SILICON

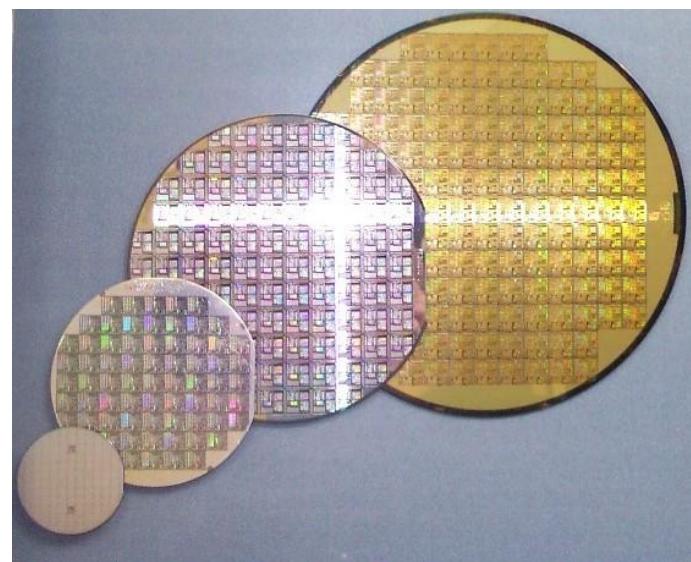
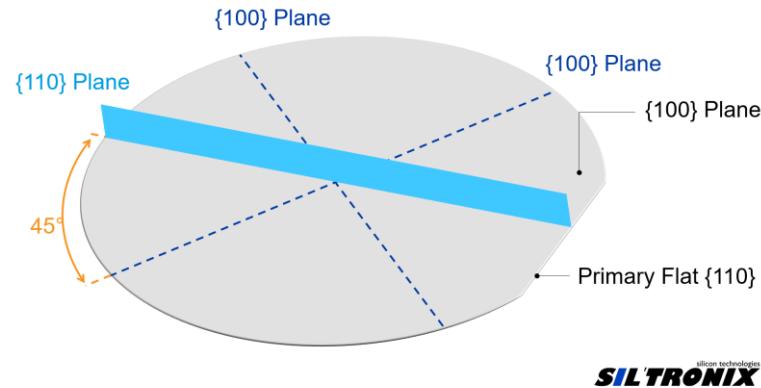


fcc structure  
**2 atoms basis**  
diamond

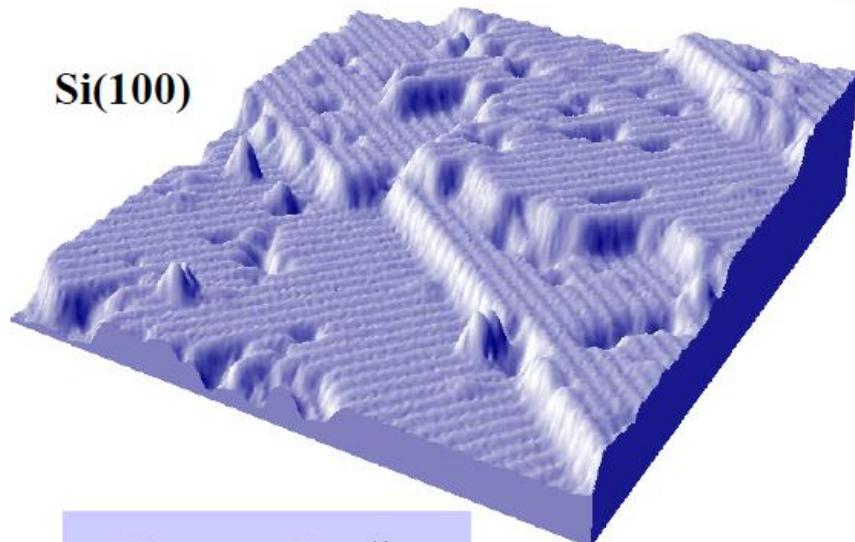
[JS mol - Silicon Crystal Planes \(tugraz.at\)](#)



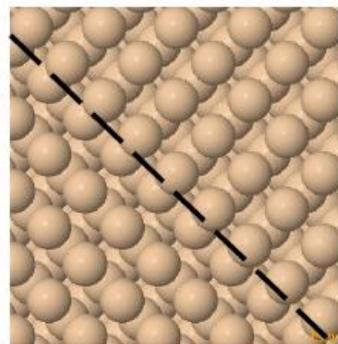
MOSFET are typically made on (100) Si wafer  
metal-oxide-semiconductor field-effect transistor



# SILICON SURFACES

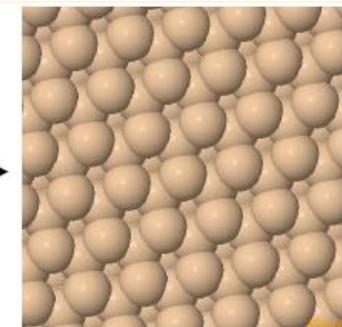


(Source: Sandia  
Nat.Labs.)

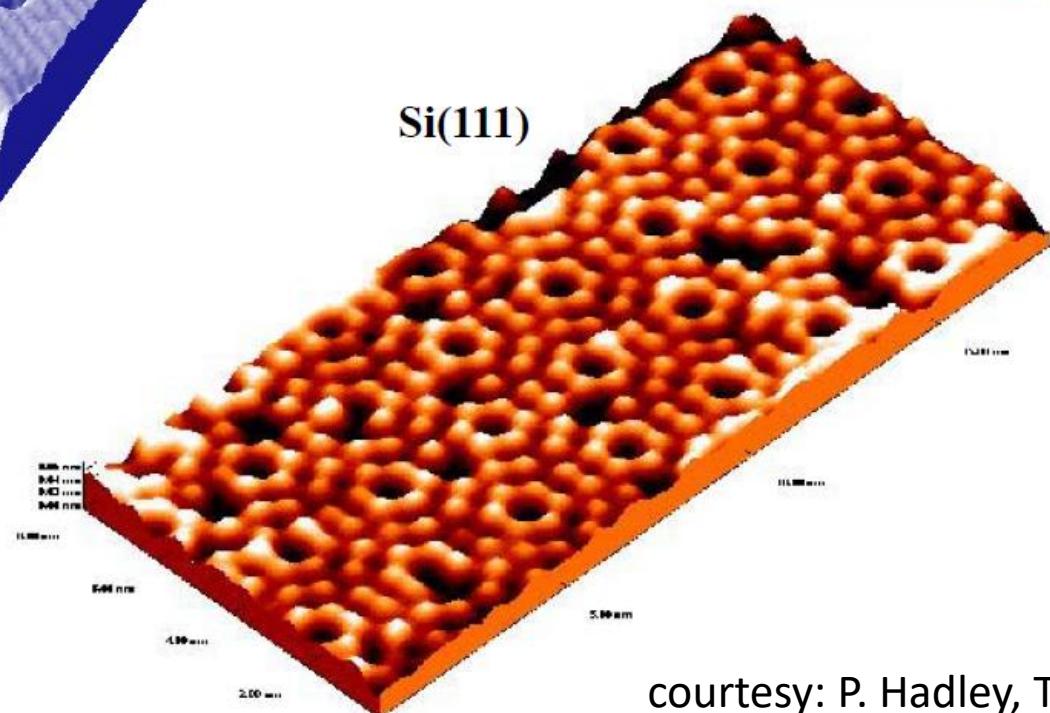


atomic  
step in  
Si(100)

unreconstructed  
Si(111) →



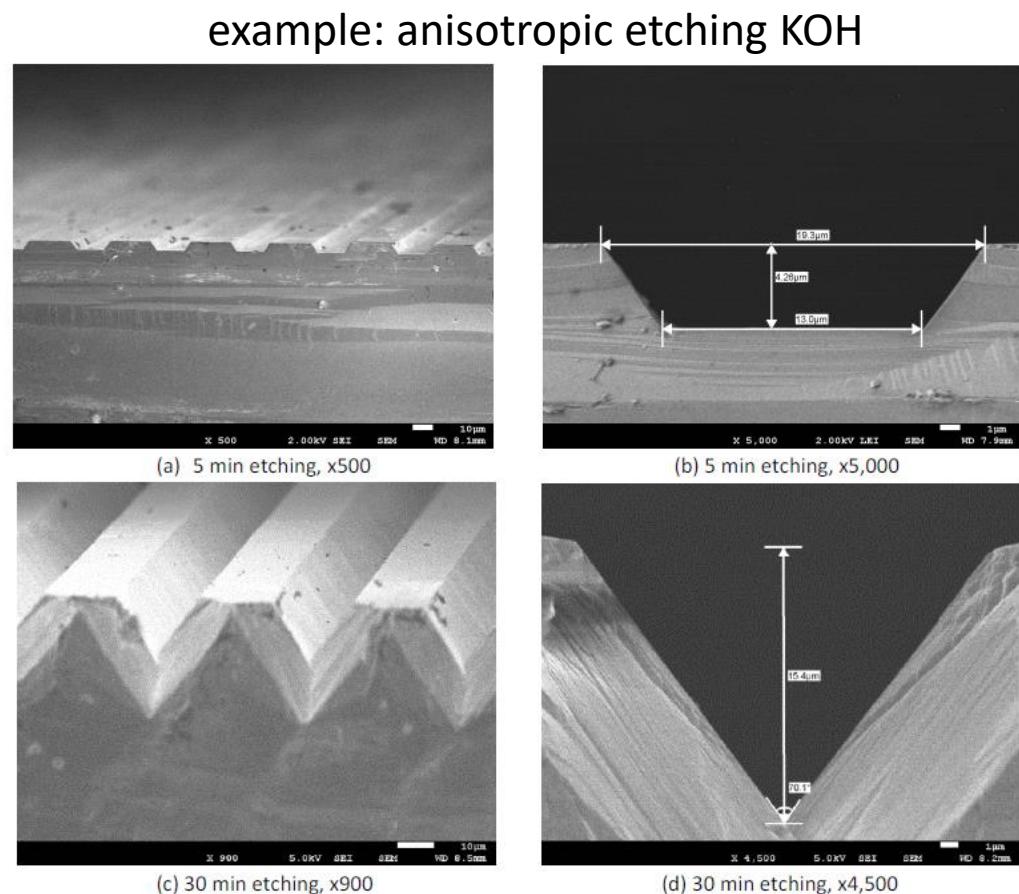
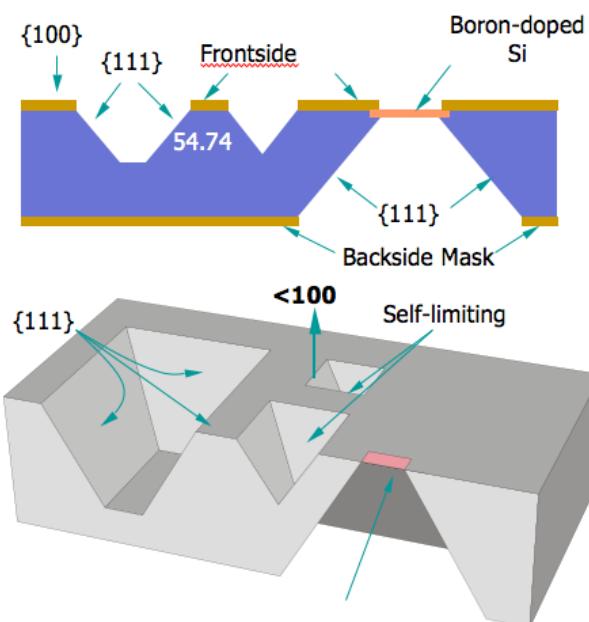
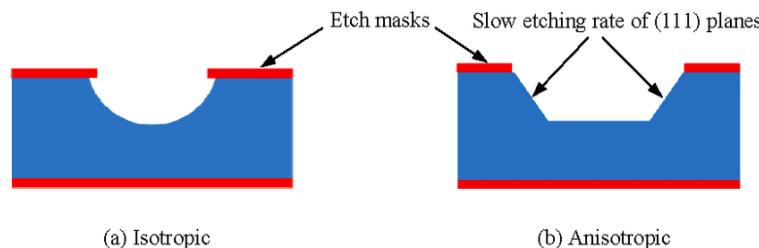
Si(111)



courtesy: P. Hadley, TUGraz

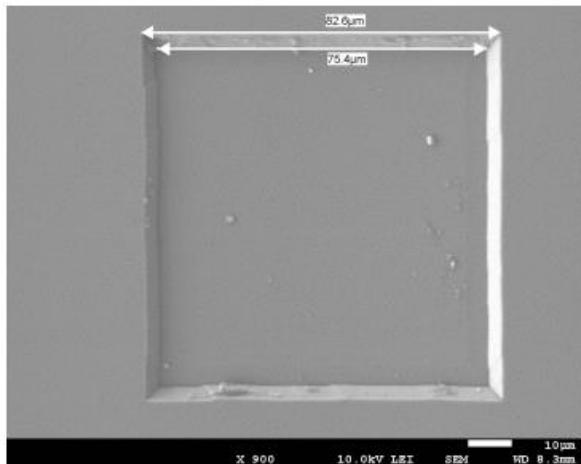
# SILICON

Anisotropic etching extremely important in MEMS and nanofabrication!

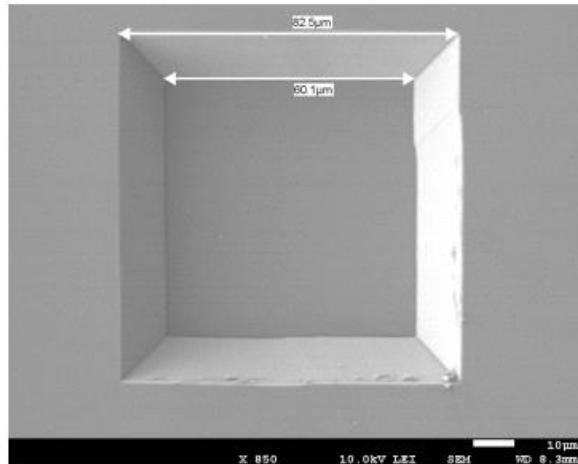


Bajwa, Inayat, "KOH etching of (100) Si wafer, No 1", *Protocols and Reports*. Paper 18.  
[https://repository.upenn.edu/scn\\_protocols/18](https://repository.upenn.edu/scn_protocols/18)

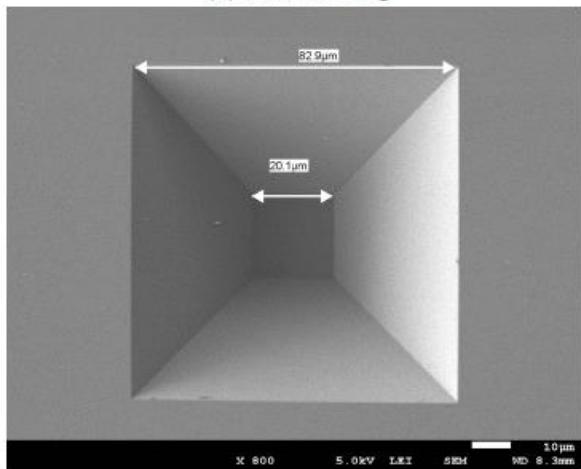
# SILICON



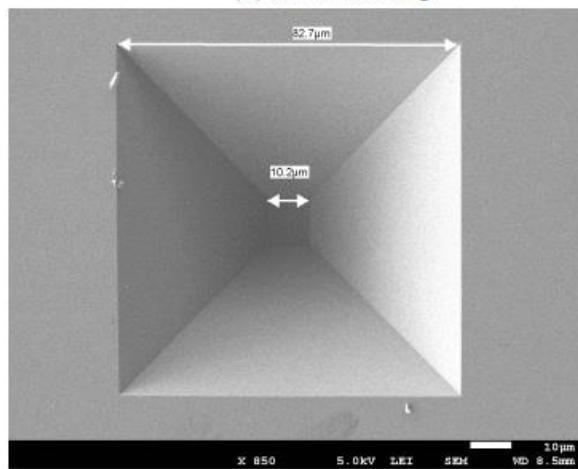
(a) 5 min etching



(b) 15 min etching



(c) 30 min etching



(d) 45 min etching

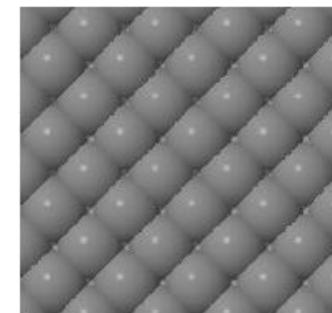
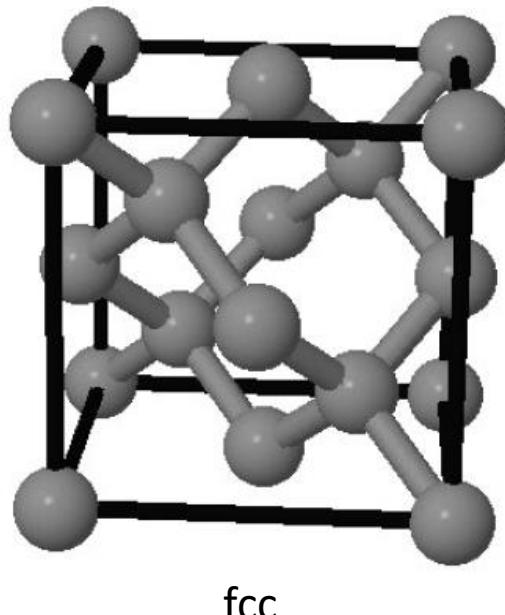
Bajwa, Inayat, "KOH etching of (100) Si wafer, No 1", *Protocols and Reports*. Paper 18.  
[https://repository.upenn.edu/scn\\_protocols/18](https://repository.upenn.edu/scn_protocols/18)

# DIAMOND

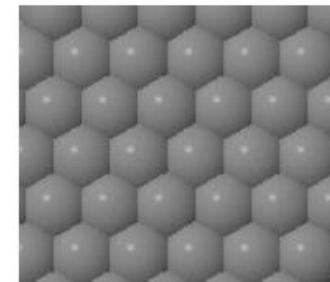
Crystal planes atomic density



[Jsmol - Diamond \(tugraz.at\)](#)



$$(100): \frac{2}{a^2}$$



$$(111): \frac{4}{\sqrt{3}a^2}$$

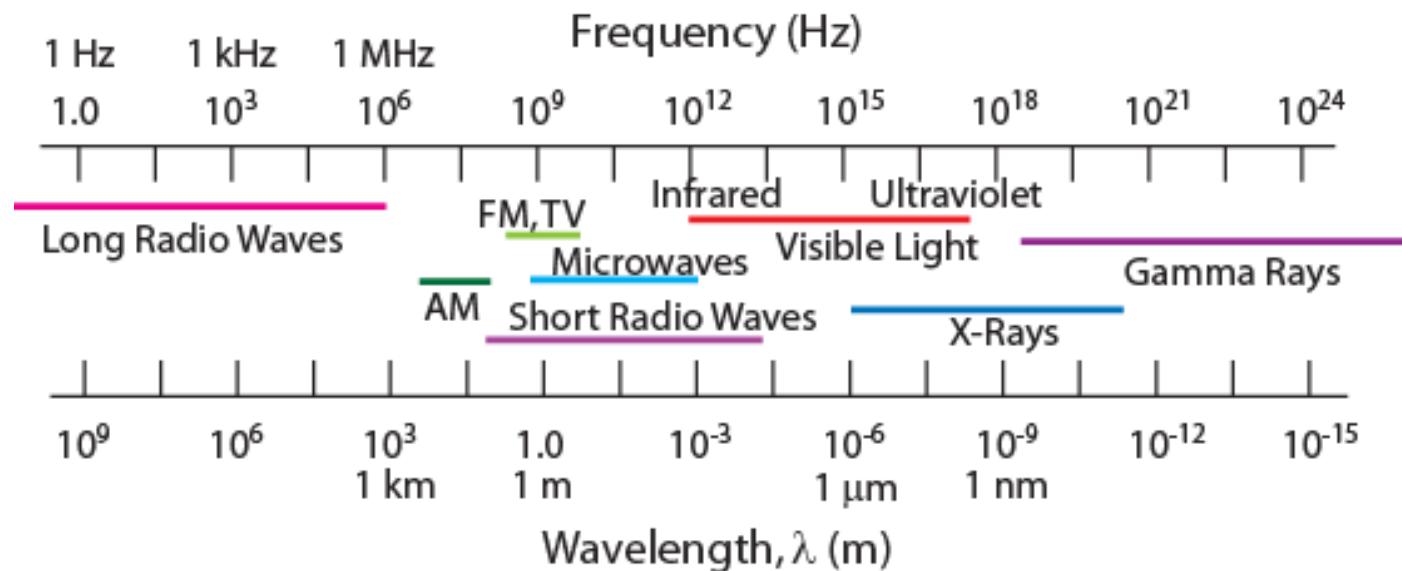


L3.6

# X-RAYS DIFFRACTION

# X-RAY DIFFRACTION

## Electromagnetic Spectrum



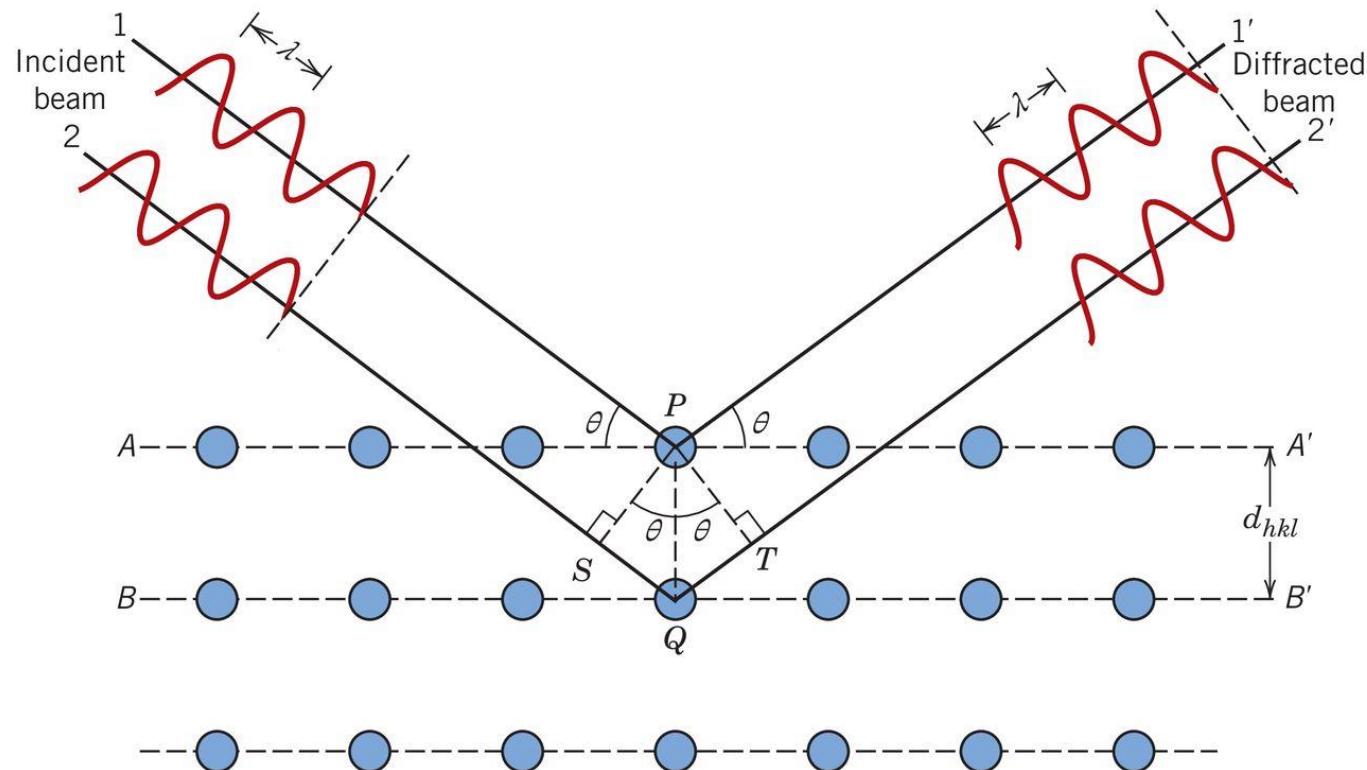
To diffract light, the diffraction grating spacing must be comparable to the light wavelength.

X-rays are diffracted by **planes of atoms**

**Interplanar spacing:** distance between parallel planes of atoms

# X-RAY DIFFRACTION

- Crystallographic planes **diffract** incoming X-rays

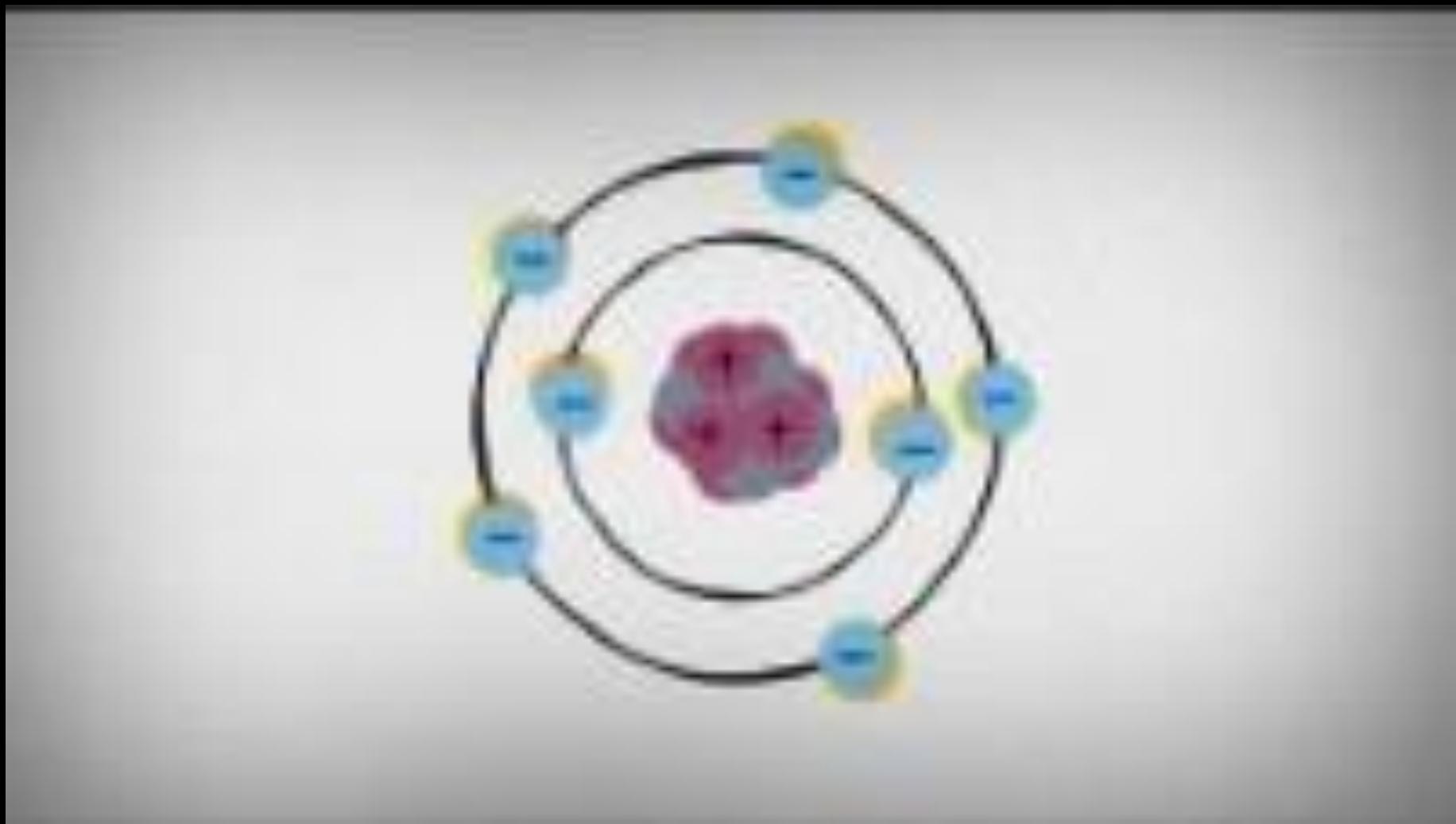


reflections must be in phase for  
**constructive interference**

$$n\lambda = 2d_{hkl} \sin\theta$$

Bragg's law

# X-RAY DIFFRACTION



YOUTUBE VIDEO (by Bruker)  
*What is X-ray Diffraction?*

(04:00)

<https://youtu.be/QHMzFUo0NL8>



# X-RAYS DIFFRACTION II

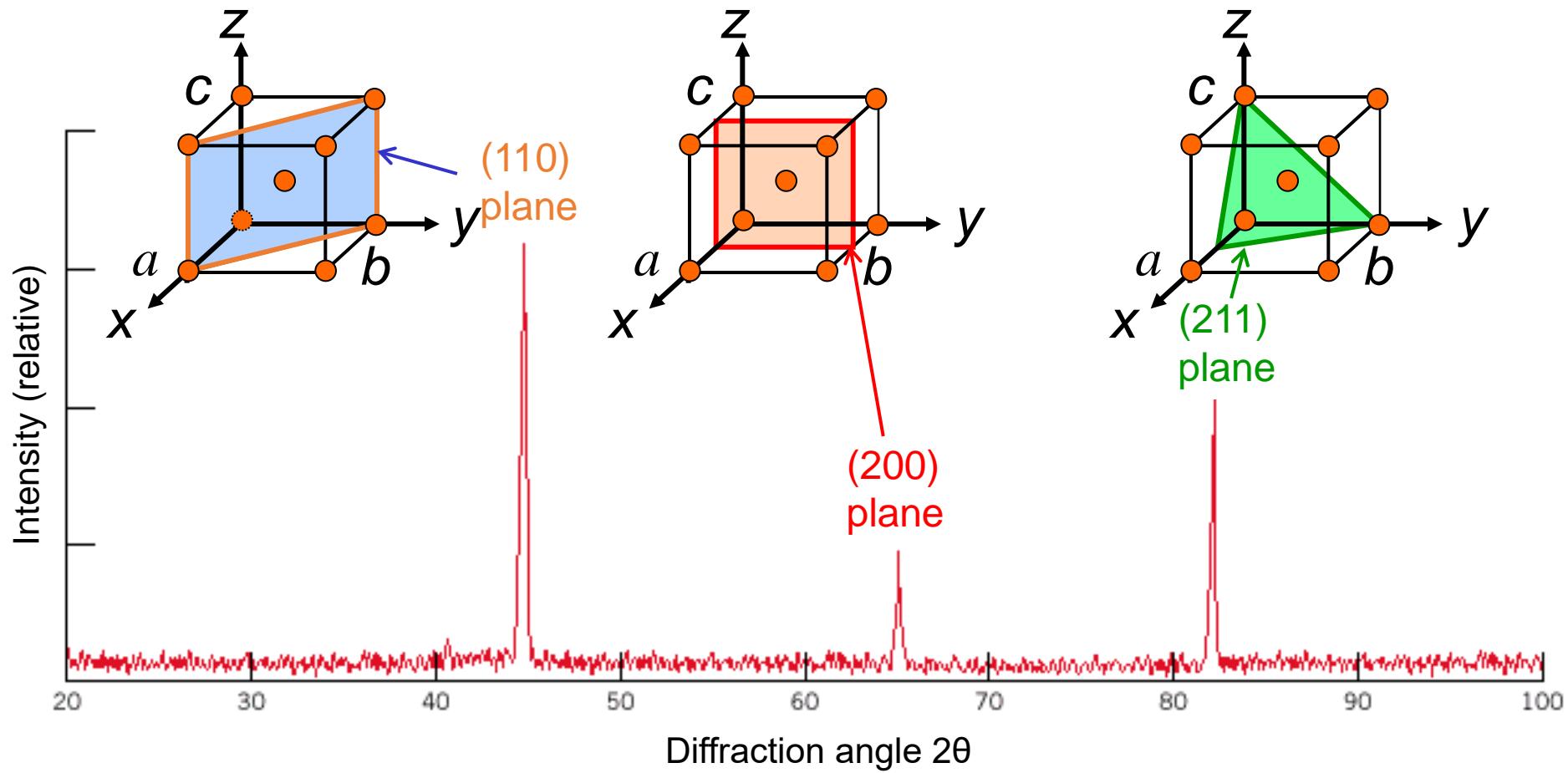
## X-Rays Diffraction for determining Atomic and Molecular Structure- JOVE

### JOVE VIDEO

JoVE Science Education Database. *Materials Engineering*. X-ray Diffraction. JoVE,  
Cambridge, MA, (2022).

<https://www.jove.com/embed/player?id=10446&t=1&s=1&fpv=1>

# X-RAY DIFFRACTION PATTERN



Diffraction pattern for polycrystalline  $\alpha$ -iron (BCC)



L3.7

# SINGLE CRYSTALS AND POLYCRYSTALLINE SOLIDS

# SINGLE CRYSTALS

- The periodic arrangement of atoms (crystal structure) extends without interruption throughout the entire specimen

Pyrite single crystal



© William D. Callister, Jr.

Si single crystal ingot



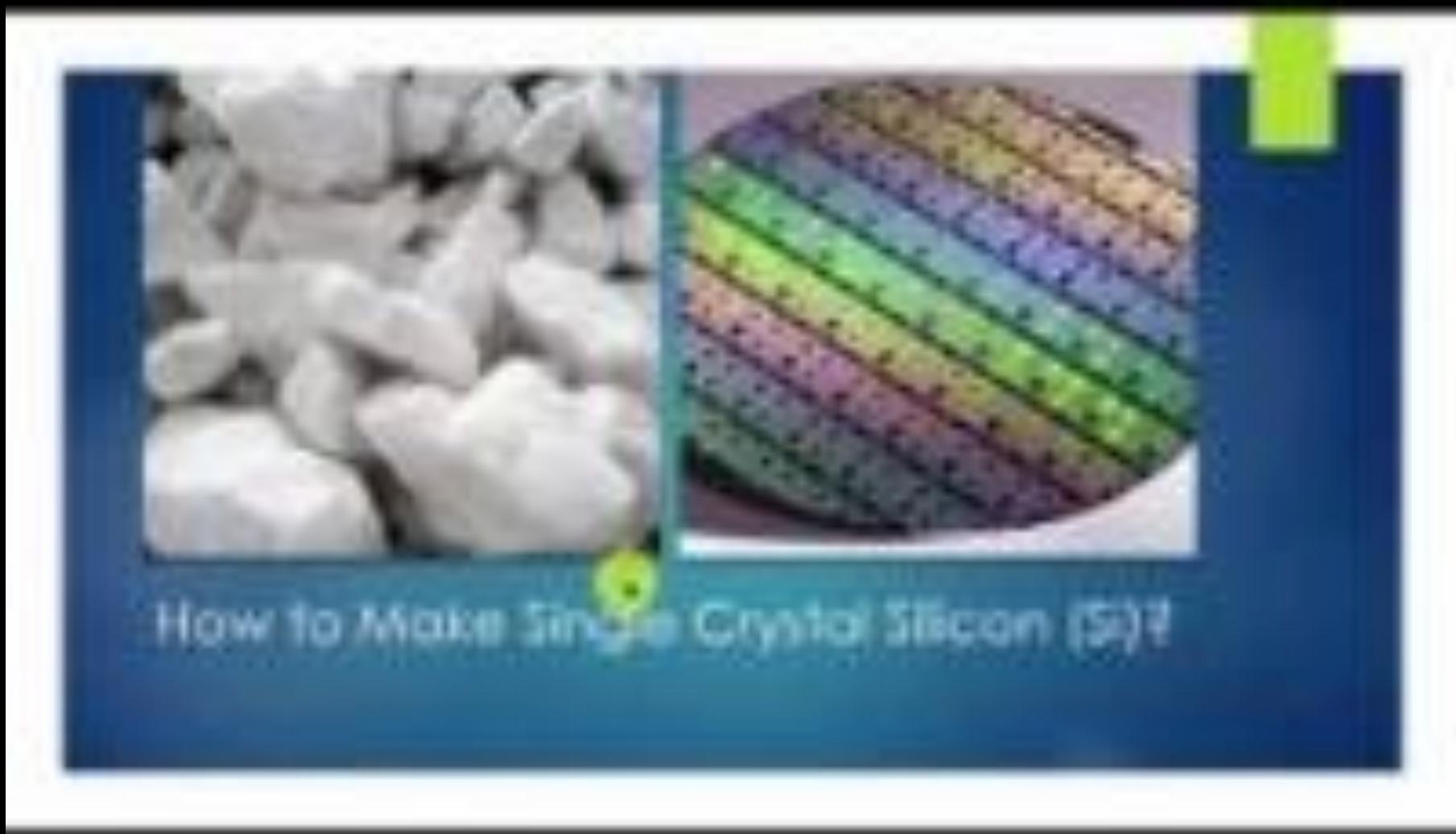
[tf.unikiel.de](http://tf.unikiel.de)

Si ingots and sliced wafers



[How to Make Si single Crystals?](#)

## SILICON SINGLE CRYSTALS



YOUTUBE VIDEO (by Bruker)  
How to Make Single Crystal Silicon? - YouTube

(04:16)

## SILICON SINGLE CRYSTALS

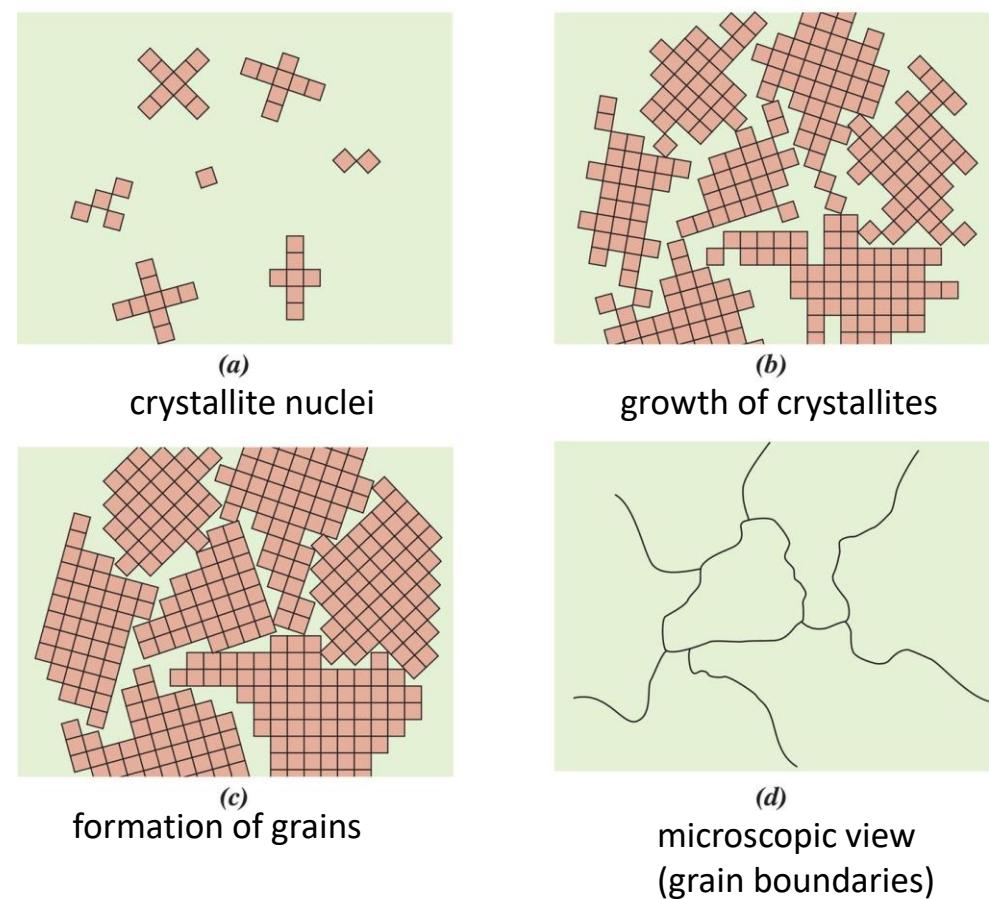
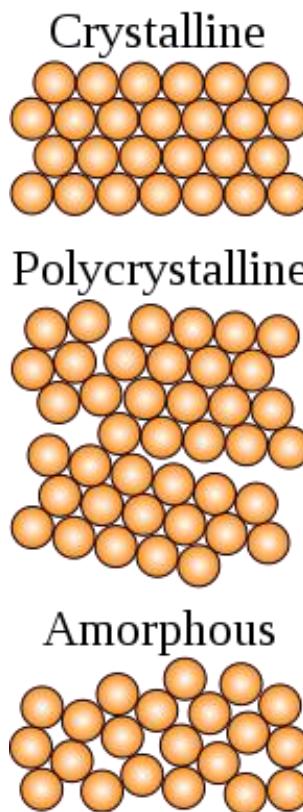


YOUTUBE VIDEO (by MicroChemicals)  
[Silicon Wafer Production - YouTube](#)

(04:16)

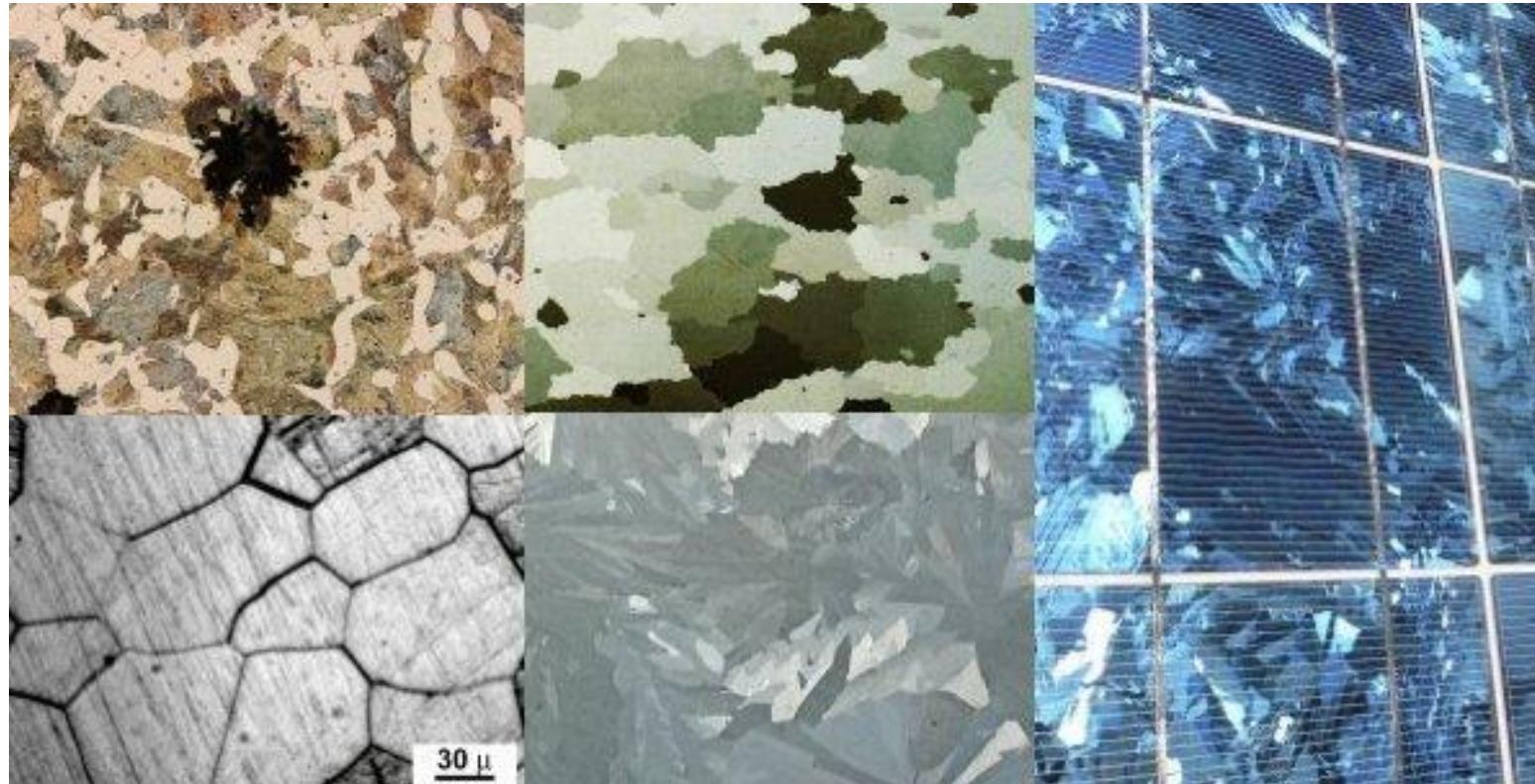
# POLYCRYSTALLINE MATERIALS

- *most* engineering materials are composed of many small single crystals: *polycrystalline*
  - each crystalline domain: *grain*. grain boundaries: contacts of domains, mismatch, defects
    - solidification of a polycrystalline solid



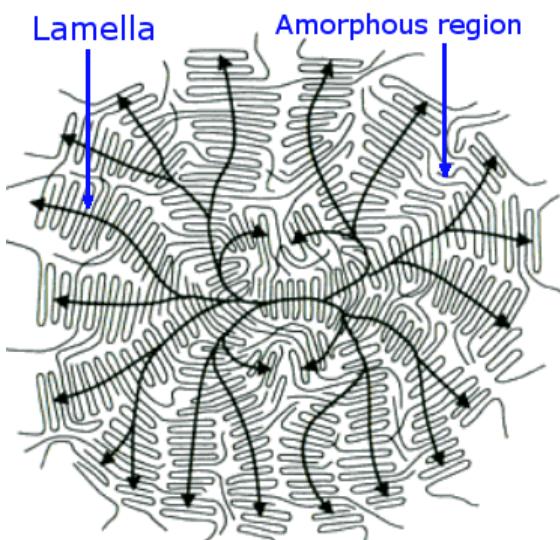
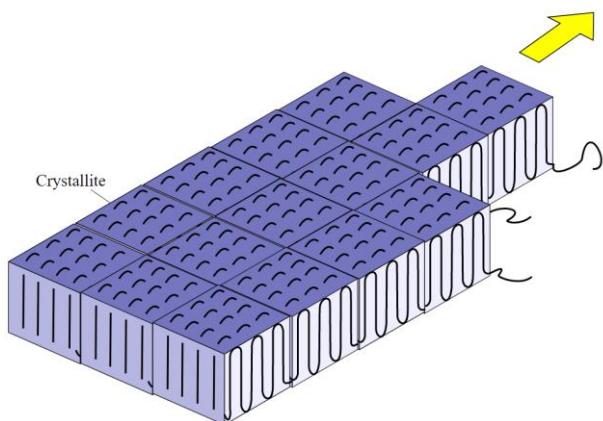
# POLYCRYSTALLINE MATERIALS

- *Most* engineering materials are composed of many small single crystals: *polycrystalline*.



# POLYCRYSTALLINE POLYMERS

## Lamellae formation in polymers

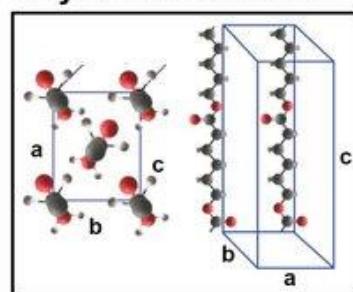


source: <https://en.wikipedia.org/>

## Spherulites (crystallites) in polycaprolactone polymer

a)

### Crystalline structure



Frontal view  
of single lamellae

Unit cell: Å

Amorphous  
region

Edge-on  
lamellae

Flat-on  
lamellae

Fibril  
(stacked  
lamellae)

Nucleation site

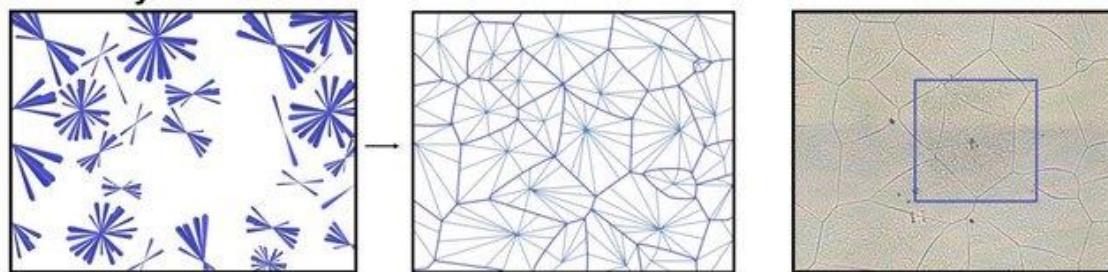
Twisted  
lamellae

Lamellae: μm

Spherulite: 100 μm

Length scale

### Polymer film



<http://dx.doi.org/10.26434/chemrxiv-2021-1hd81-v2>

# SUMMARY

- Atoms may assemble into **crystalline** (ordered) or **amorphous** (disordered) structures
- Common crystal structures are **FCC**, **BCC**, and **HCP**.
- We can calculate the theoretical **density** of a metal, given its **crystal structure**, **atomic weight**, and **unit cell lattice parameters**
- Some materials can have more than one crystal structure:  
**polymorphism** (or **allotropy**)
- **Crystallographic points**, **directions** and **planes**: indexing schemes
- **Atomic densities** are related to crystallographic directions and planes

# SUMMARY

- X-ray diffraction is used for crystal structure and interplanar spacing determinations
- Materials can exist as single crystals or polycrystalline
- For most single crystals, properties vary with crystallographic orientation:  
anisotropic
- For polycrystalline materials having randomly oriented grains, properties are independent of crystallographic orientation  
isotropic

# SUMMARY L3

- L3.1 • Crystalline solids, Definitions
- L3.2 • Lattices, Unit cells --> Crystal Structures
- L3.3 • Crystal Structures, Packing of Atoms
- L3.4 • Density
- L3.5 • Crystallographic Planes
- L3.6 • X-rays diffraction: determination of crystal structure
- L3.7 • Single Crystals and Polycrystalline solids



# READINGS

## READINGS:

- Callister Rethwisch – Chapter 3



# 3D STRUCTURE VIEWERS

[OPEN SOURCE MOLECULE VIEWER JSmol molecule viewer \(tugraz.at\)](#)

[Interactive 3D Chemistry Animations — ChemTube3D](#)



# ADDITIONAL RESOURCES 1

Video series course  
on YOUTUBE

[THE FASCINATION OF CRYSTALS AND SYMMETRY](#)

7 CHAPTERS

by F. Hoffmann – Hamburg University

ADDITIONAL MATERIAL; SLIDES; NOTES of this course available at  
[The Fascination of Crystals and Symmetry | Crystals are fascinating objects. \(wordpress.com\)](#)



# ADDITIONAL RESOURCES 2

Videos  
on YOUTUBE

more on FCC structures

[FCC structure - Texas A&M: Intro to Materials](#)

by P. Shamberger – Texas A&M Univ.

more on Single Crystals, Polycrystalline, Amorphous materials

[Single Crystals, Polycrystalline, Amorphous - Texas A&M: Intro to Materials](#)

by P. Shamberger – Texas A&M Univ.

more on Silicon Single Crystal

[How to make a Silicon single crystal](#)

by Fiber Optics For Sale Co.