Session 2: Solid State Physics

Crystal

Outline

- Introduction
  - Course information
  - Technology
  - State of matter
  - Micro/macro -oscopic aspects of matter
- Crystal
  - Bravis lattice
  - Primitive unit cell, unit vectors, Wigner-Seitz unit cell
  - Basis, Crystal
  - Example: Graphene
- Cubic Lattices
  - SC, BCC, FCC, Zinc Blende
- Other
- Symmetry
- Miller Indices

Introduction – Text Books

Streetman,
Solid State Electronic Devices

Pierret,
Semiconductor Device Fundamentals

Yang,
Microelectronic Devices

Muller,
Device Electronics for Integrated Circuits

Introduction – Course Information

Course homepage:
http://ee.sharif.edu/~sarvari/Teaching.html

Refresh the page!

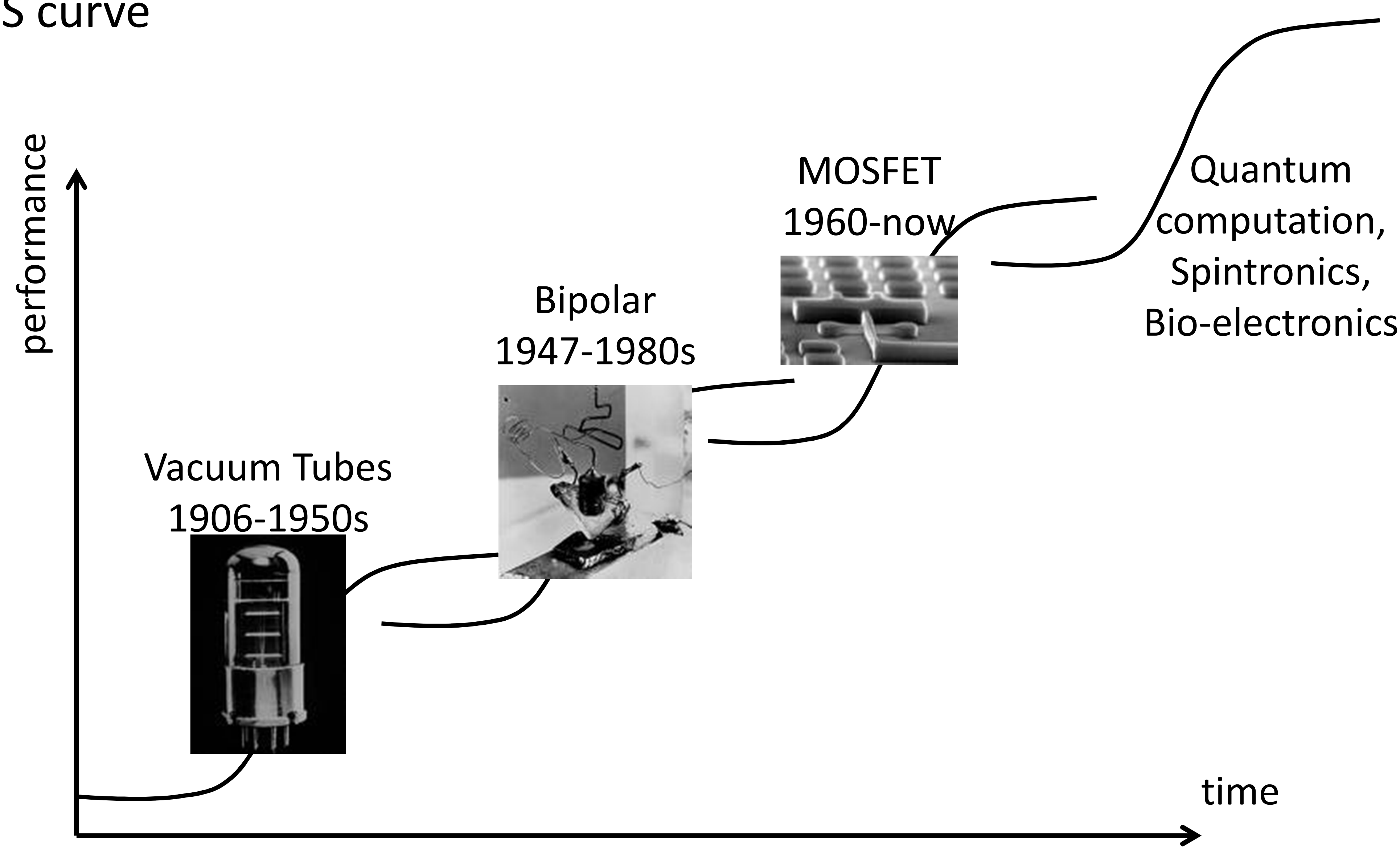
Grading (tentative):
2-MidTerms (40%) + HW & Quizzes (20%) + Final (40%)

?, ?

http://cw.sharif.edu/

Technology Challenges

S curve



Abbreviated Periodic Table

Elements:
Si, Ge, C

Binary:
III-V: GaAs , Inp
II-VI: ZnSe (zinc selenide) , CdTe (cadmium telluride)
IV-IV: SiC
IV-VI: PbS (lead sulphide)

Alloys:
ternary: Al_{1-x} Ga_{1-x} As , Hg_{1-x} Cd_x Te
Quaternary: In_{1-x-y} Ga_x Al_y As , In_{1-x} Ga_x As_{1-y} P_y

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

Not all combinations possible:
lattice mismatch, room temp. instability, etc. are concerns

States of Matter

? Why Solid State?

1. **Solid:** density ~ 10^{22} /cm^3
   - 1. a: Crystal: long range order (lattice + basis) {Ex: Epitaxial silicon and diamond}
   - 1. b: Polycrystal: short range order (µm ~ 10µm) {Ex: Most metals (Al, Cu) Ploy-Si}
   - 1. c: Amorphous: no order {Example: Glasses like SiO2}

2. **Liquids:** no order, takes the shape of the container, weak bounds; density ~ 10^{19} /cm^3

3. **Gases:** no order, no bounds between molecules

4. **Liquid crystals:** atoms mobile, type of long range order Applications: LCDs

5. **Plasma:** Ionized gas/liquid {Ex: Sun, Aurora, Lightning, (RIE, Sputtering, PECVD)}

Why WE Should care?

Isn't it for physics / Chemistry / Material Science Department?

1. Solid: density ~ 10^{22} /cm^3

a: Crystal: long range order (lattice + basis)

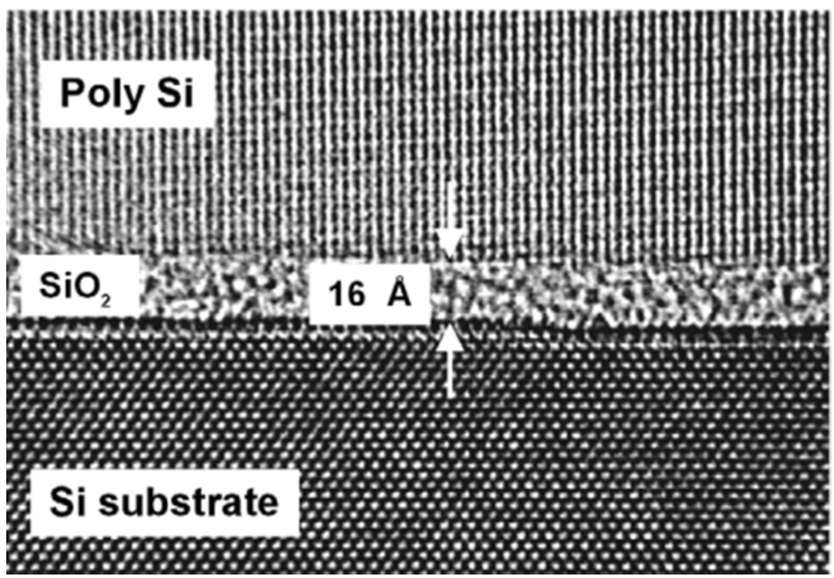
{Example: Epitaxial silicon and diamond}

b: Polycrystalline: short range order (µm~10µm)

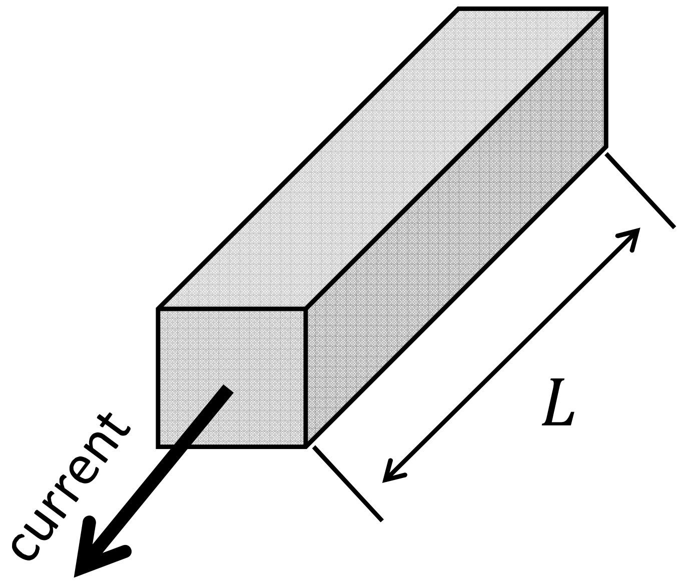
{Example: Most metals (Al, Cu) Ploy-Si}

c: Amorphous: no order

{Example: Glasses like SiO_2}



Resistivity



Ohm's law

$$R = \frac{V}{I} \quad \rightarrow \quad \rho = R\frac{A}{L}$$ resistivity

Resistivity is characteristic of the material

Art of VLSI design is:
to put together materials with different resistivity's next to each other to perform a certain task.

Conductor

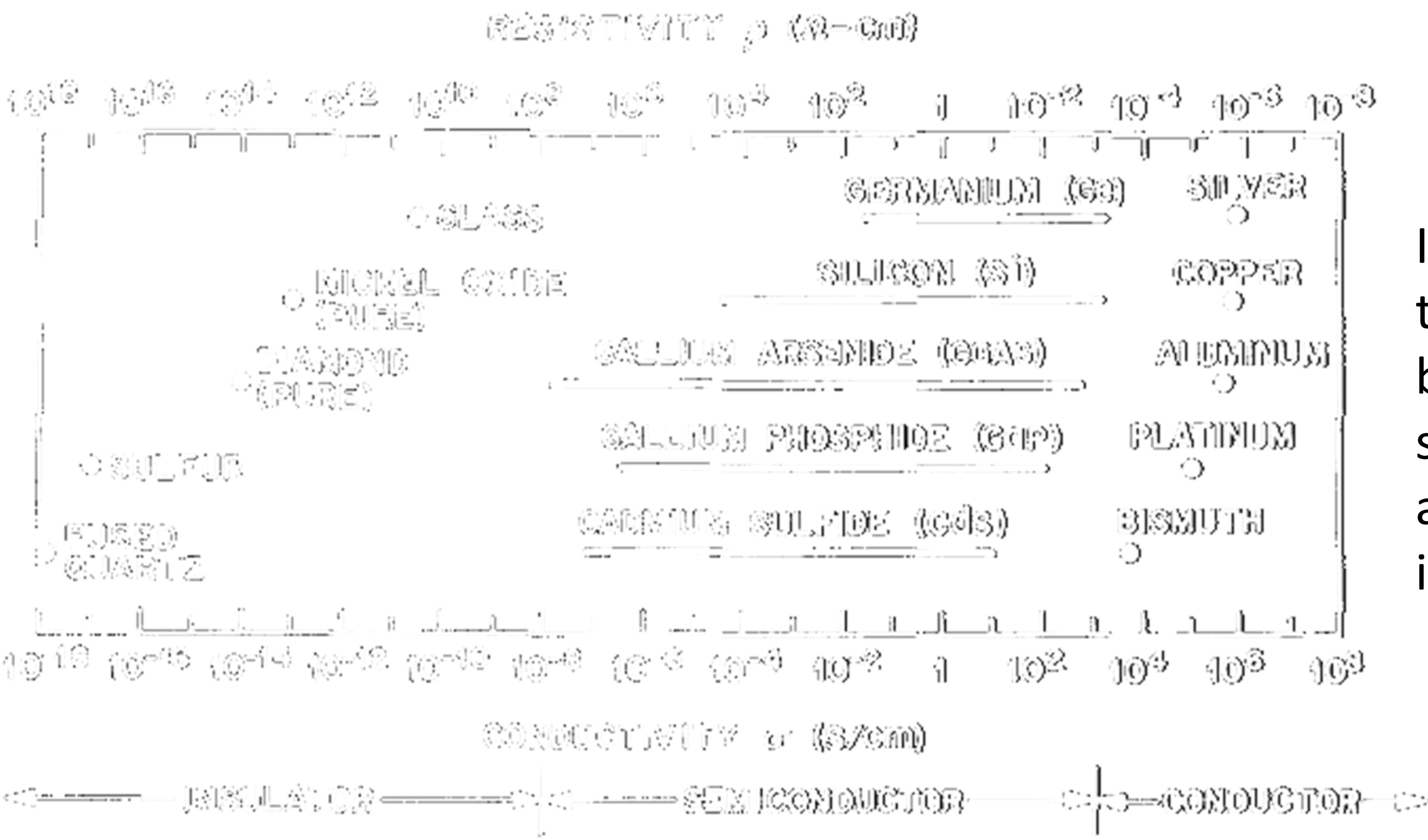
Al , Cu ⟷ SiO_2

Insulator

$\rho_{Al} \approx 10^{-6}\ [\Omega cm]$

$\rho_{SiO_2} \approx 10^{16}\ [\Omega cm]$

Semiconductors



?

Is the "resistivity" the only difference between semiconductors and conductor / insulators ?

In semiconductors: conductivity is controllable

In conductors: carriers are "electrons"
In semiconductors: carriers are "electrons" + "holes"

A Little History – Crystal Structure

Solids tend to form ordered crystals

Rock Salt

Rock Candy

Mineralogists have been familiar with crystal structures since 18th century.
1912: Diffraction of x-rays by a periodic array.
Today : Condensed matter physics long way to go .....

Properties (mechanical, electrical, optical and thermal properties all affected) of solids depends on their structure

Crystal Lattice

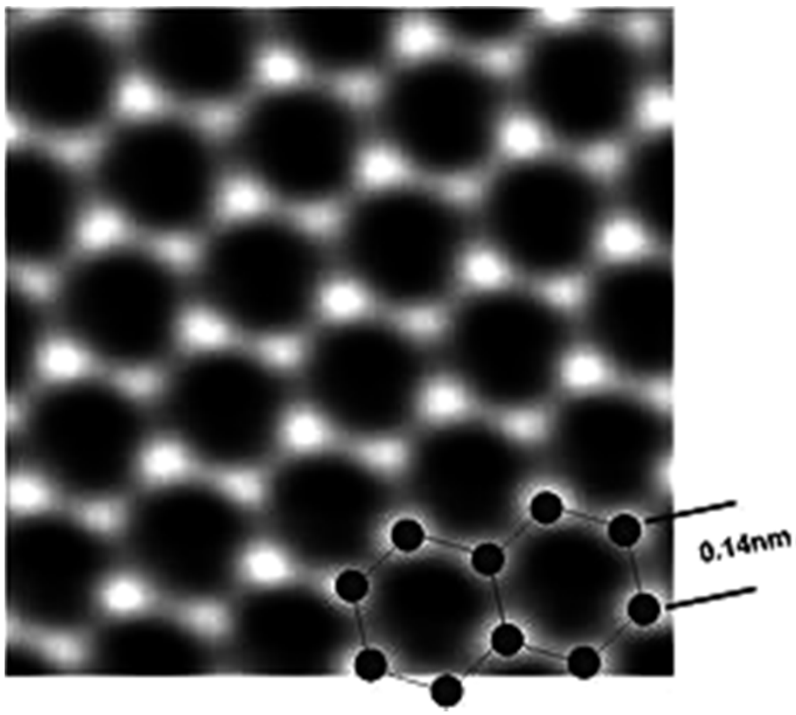
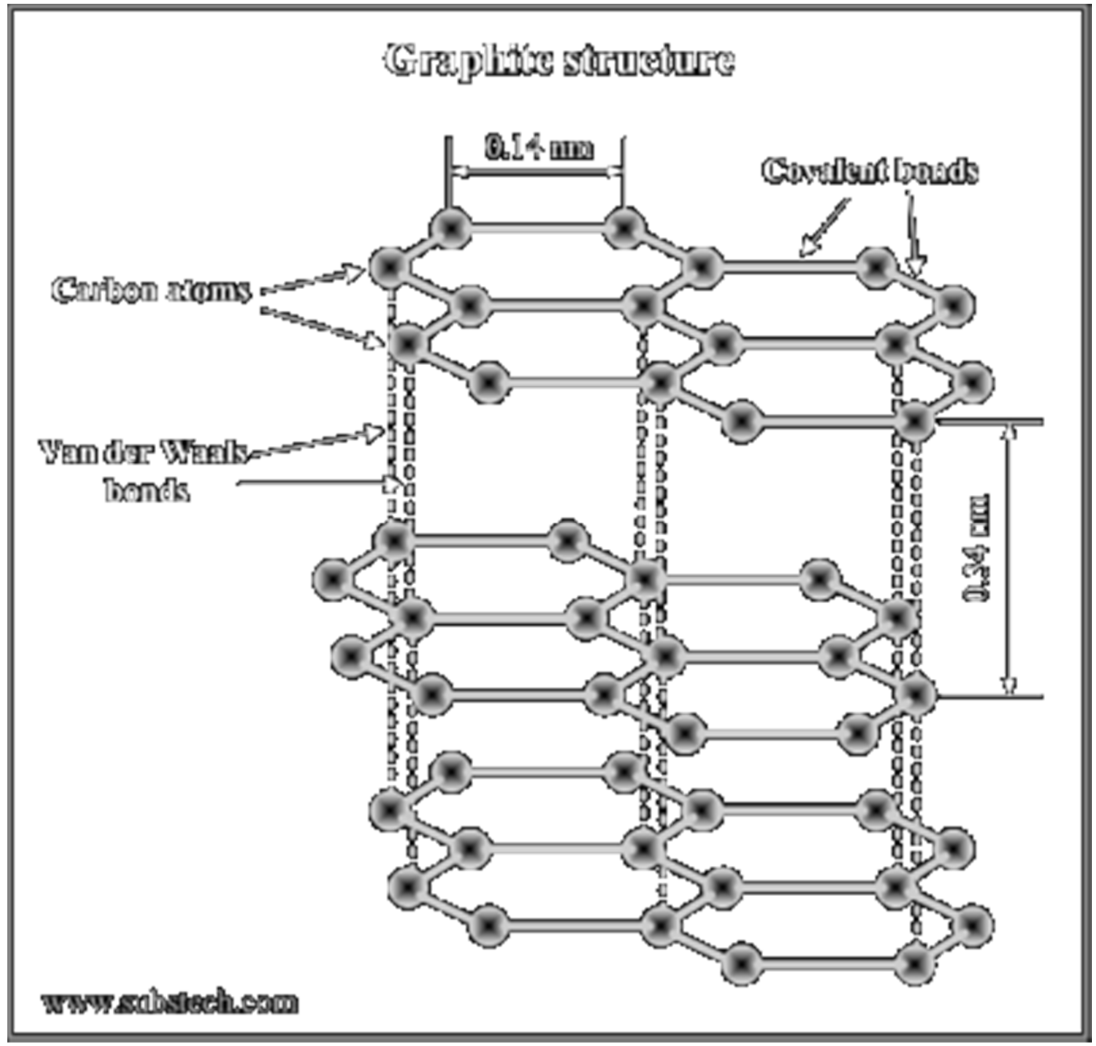
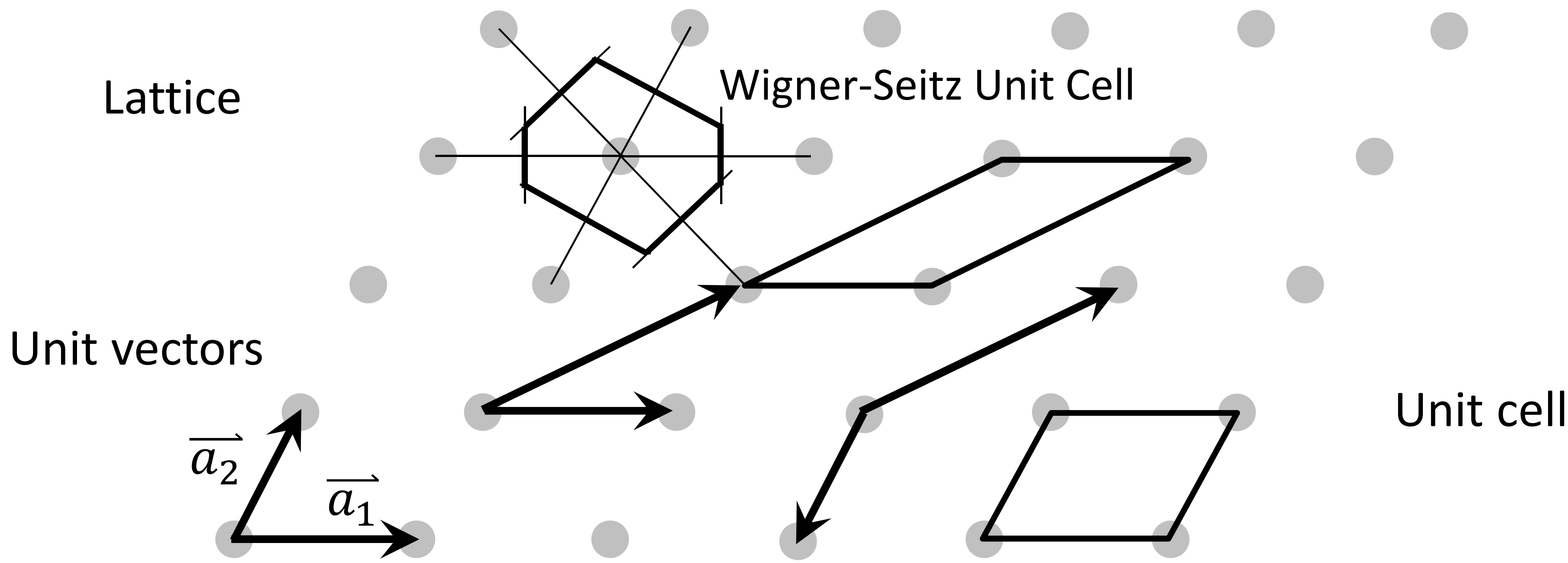


Image of graphene in a transmission electron microscope.



Bravais Lattice

Ideal Crystal: Infinite repetition of identical structural units in space.

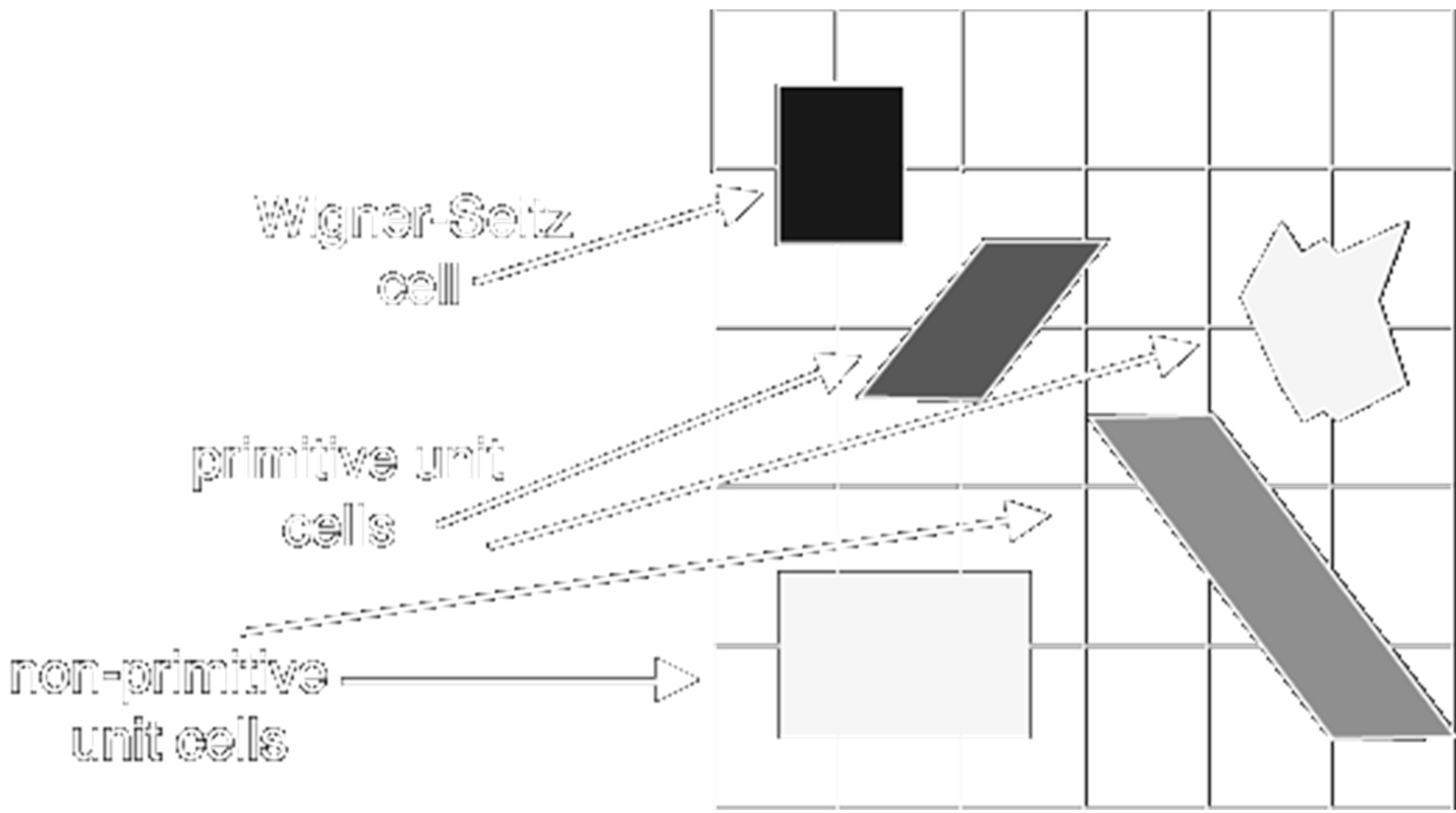


$$\vec{R} = n_1\overrightarrow{a_1} + n_2\overrightarrow{a_2}$$

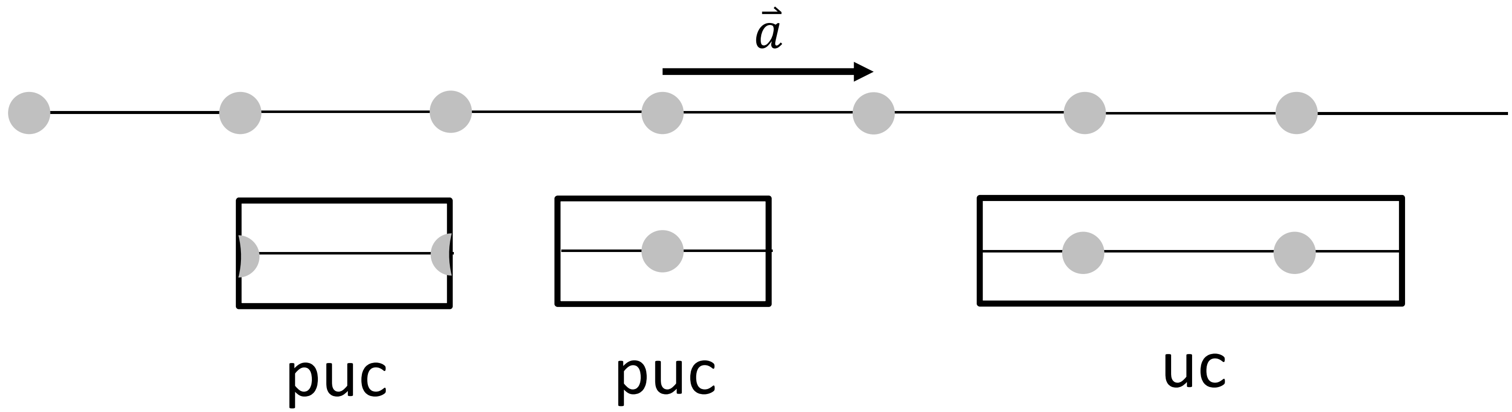
Bravais lattice: is the set of points defined by $\vec{R} = n_1\overrightarrow{a_1} + n_2\overrightarrow{a_2}$ as n_i is integer.
Shortest possible $\overrightarrow{a_1}$ gives us primitive vectors.
The volume cell enclosed by the primitive vectors is called the primitive unit cell.

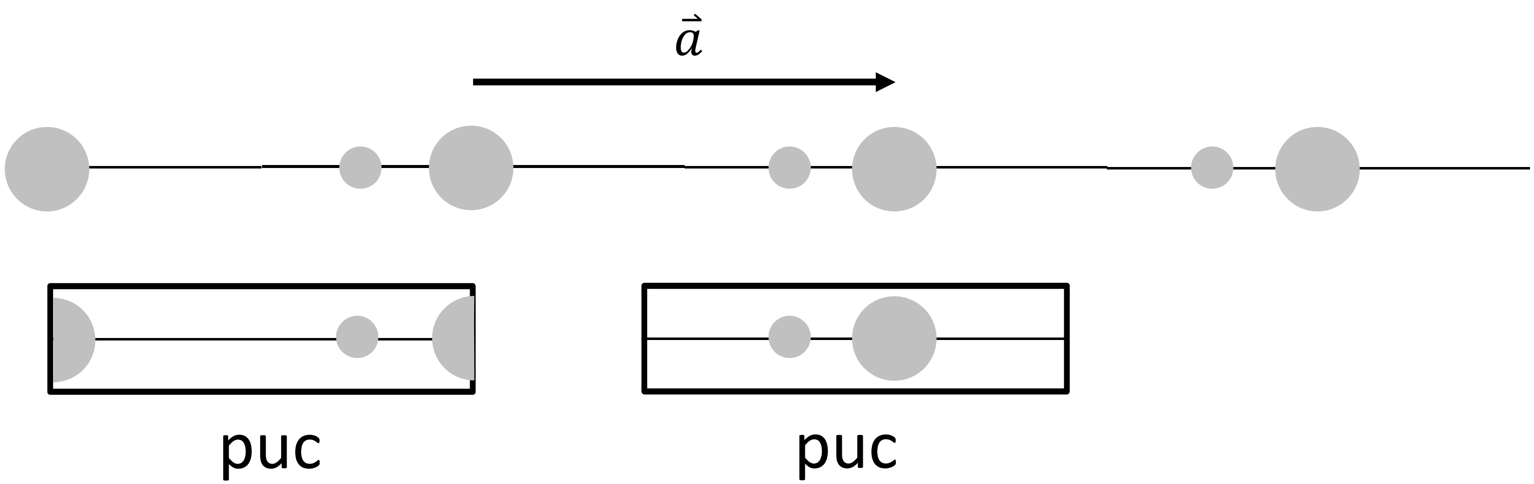
Crystal structure = Lattice + Basis

Unit cells / Wigner-Seitz cell for a rectangular 2-D lattice



1-D Lattices

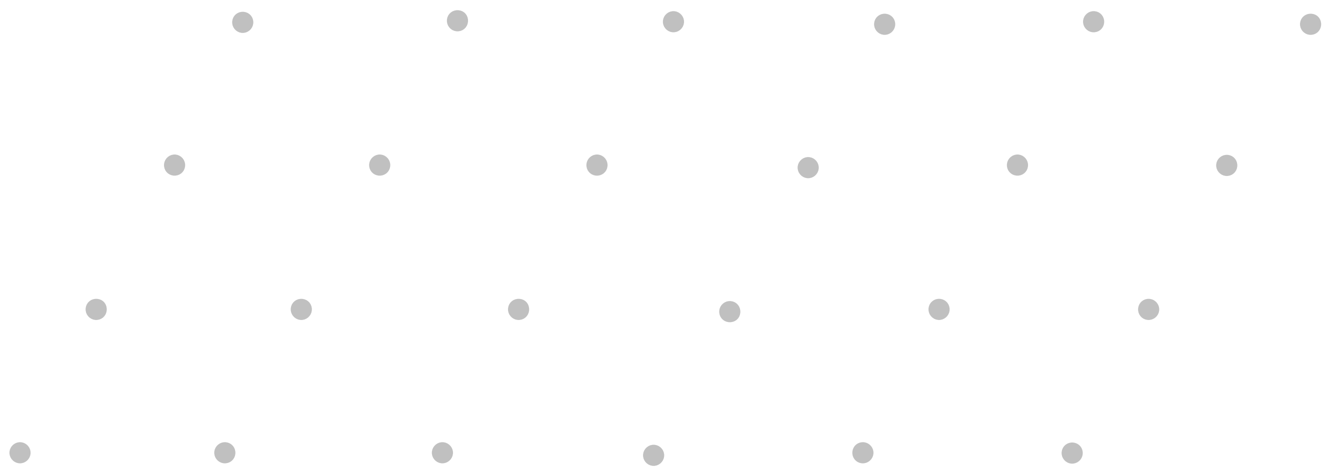




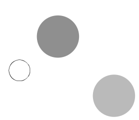
Crystal structure = Lattice + Basis

Ideal Crystal: Infinite repetition of identical structural units in space.

Lattice



basis



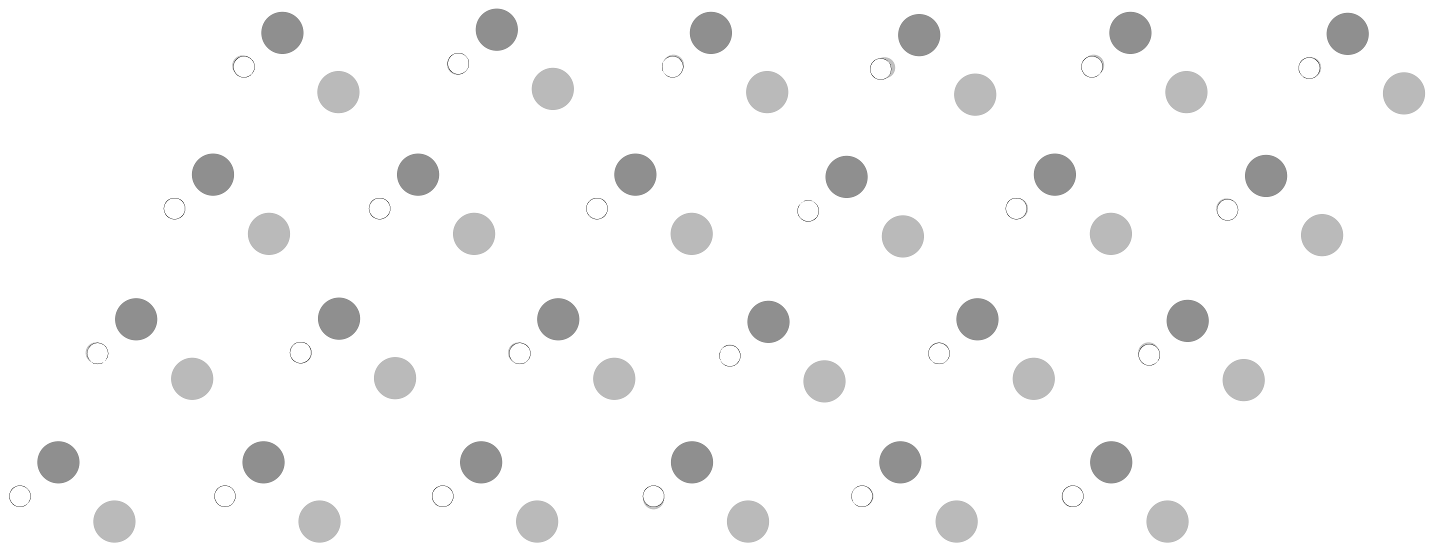
The basis consists of the simplest arrangement of atoms which is repeated at every point in the lattice to build up the crystal structure

Crystal structure = Lattice + Basis

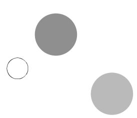
Crystal structure = Lattice + Basis

Ideal Crystal: Infinite repetition of identical structural units in space.

Lattice



basis



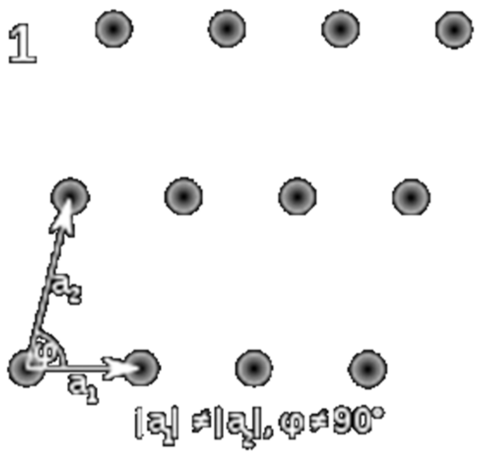
crystal

Crystal structure = Lattice + Basis

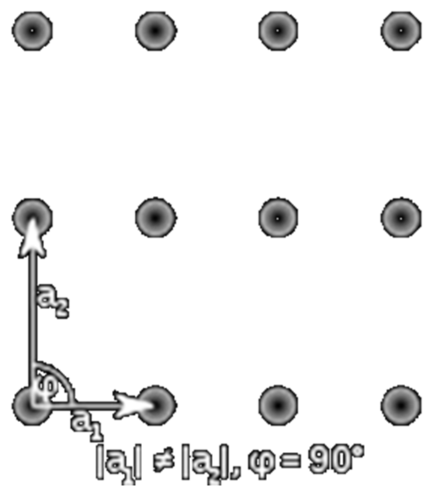
Bravais Lattices in 2D

There are only 5 Bravais lattices in 2D

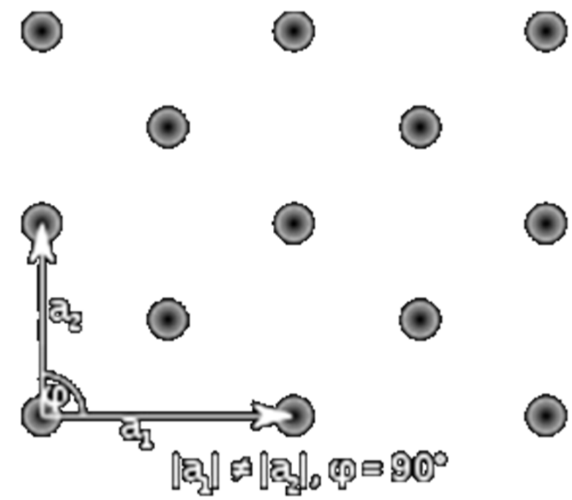
Oblique



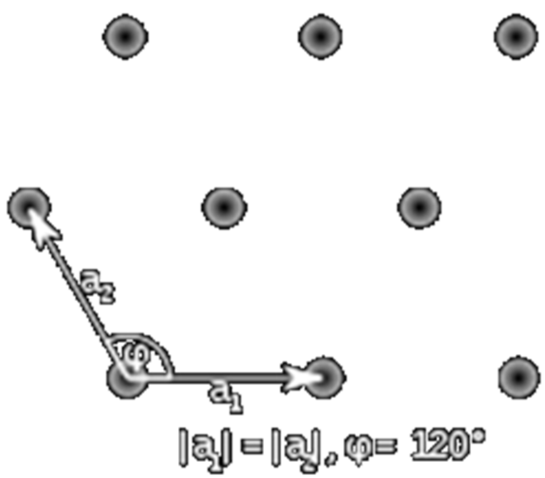
Rectangular



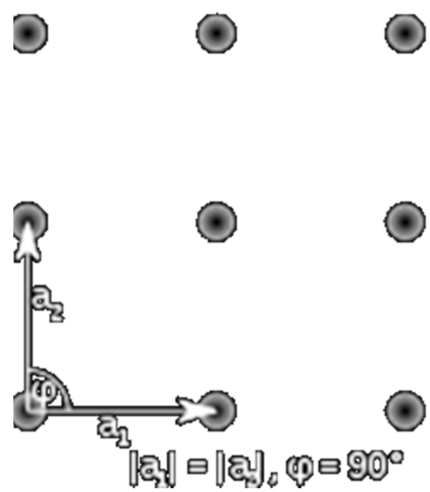
Centered Rectangular



Hexagonal



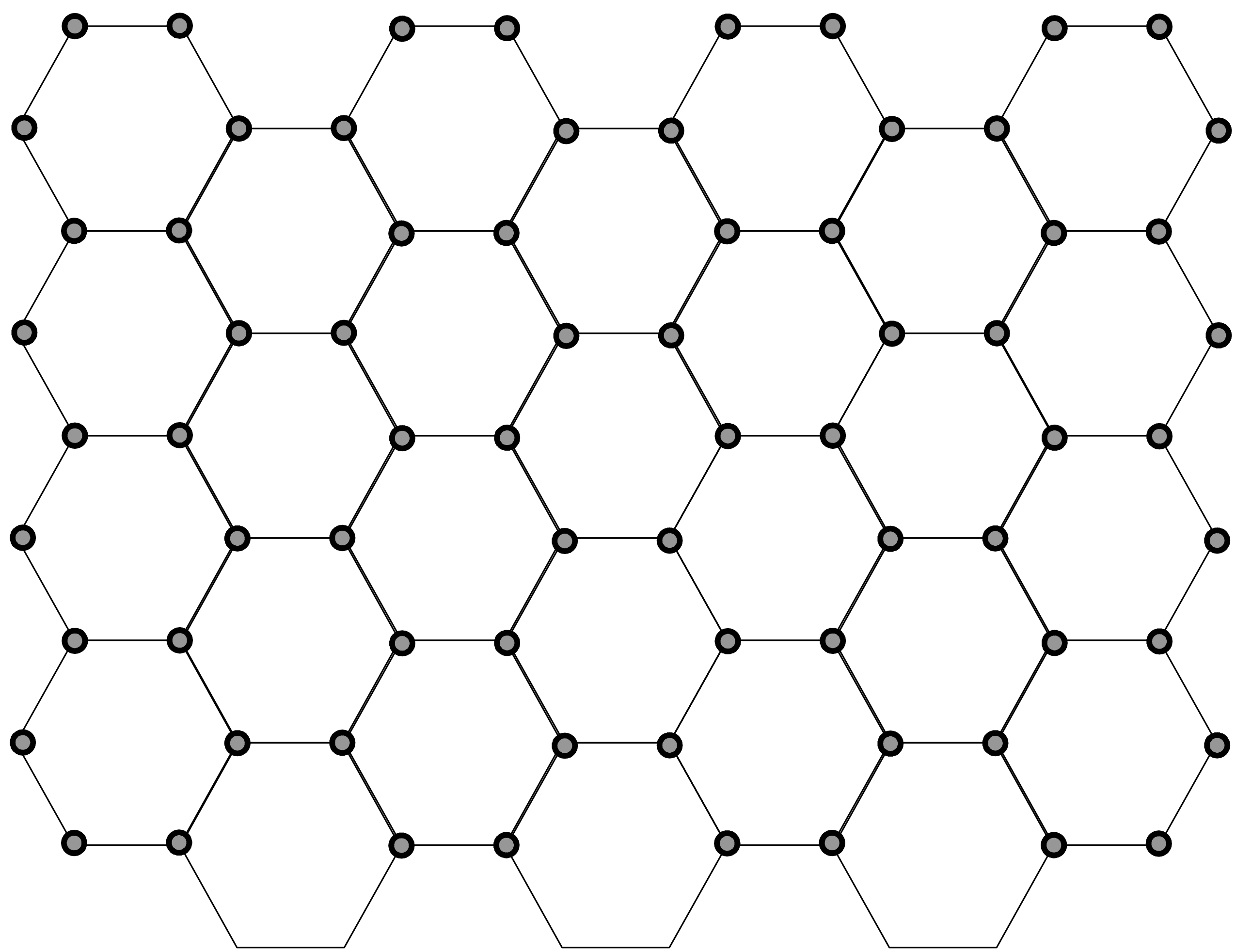
Square



Crystal Lattice, Graphene

Example: Graphene

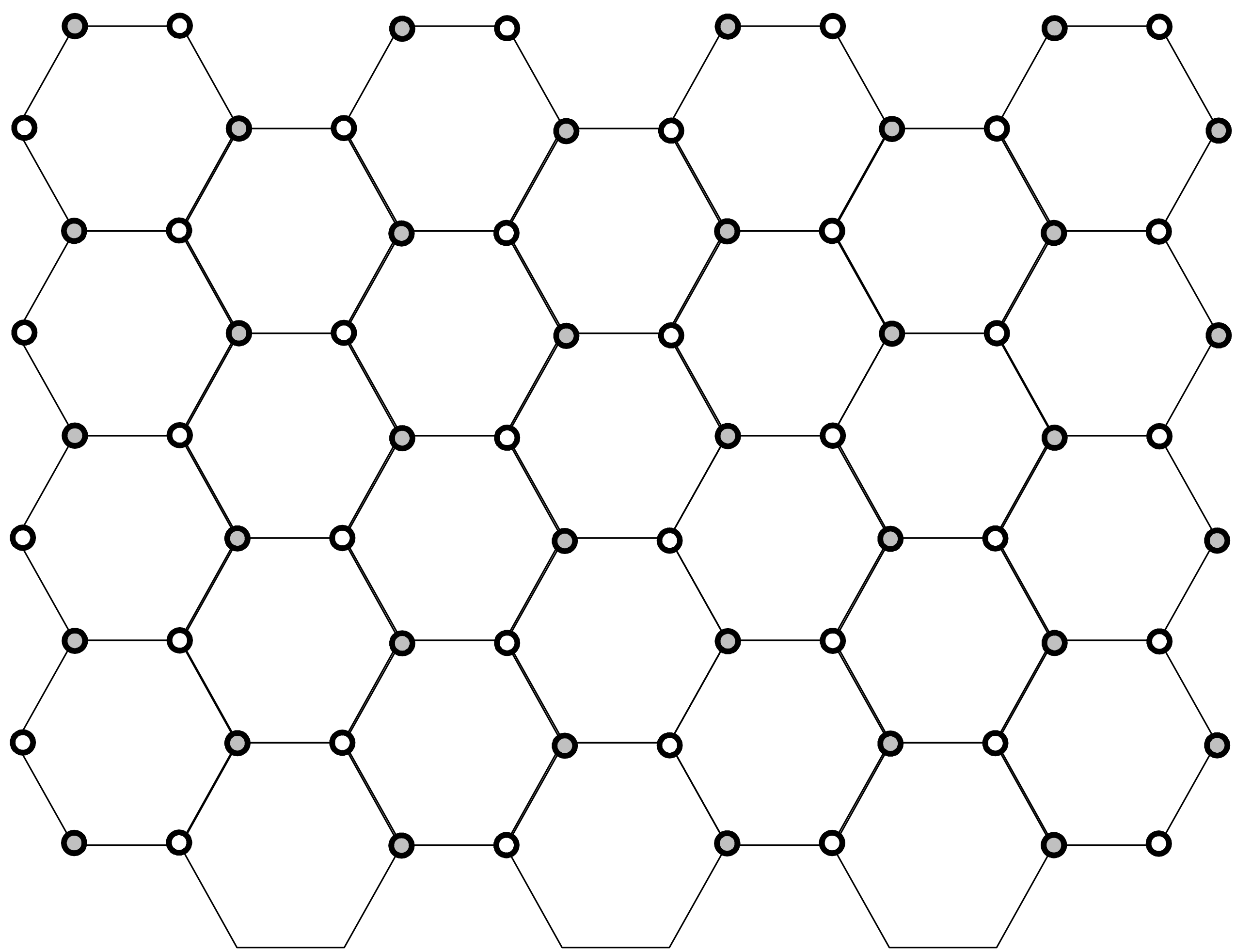
Honeycomb structure



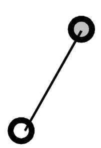
Crystal Lattice, Graphene

Example: Graphene

Honeycomb structure



basis



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Example: Graphene

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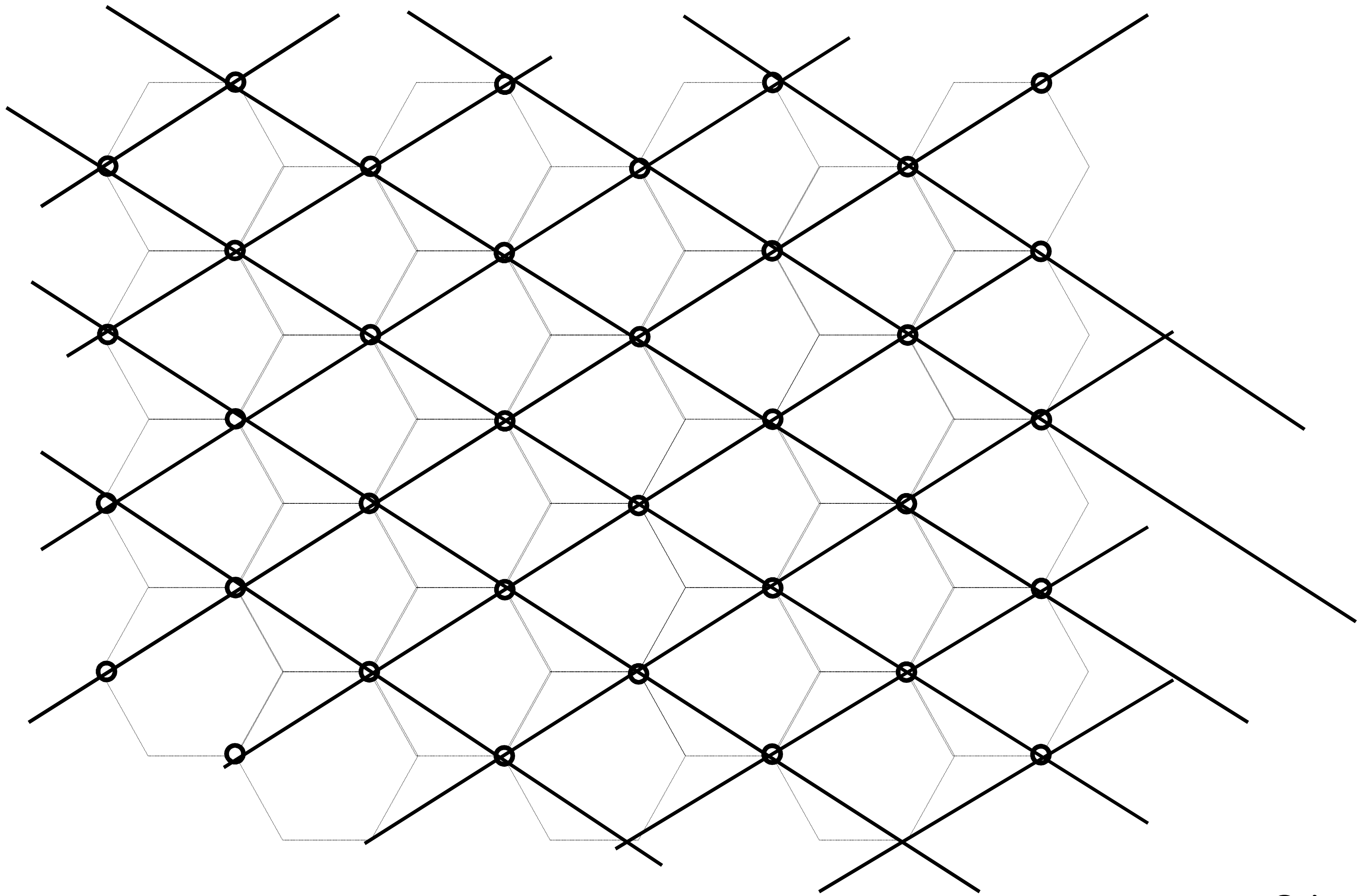
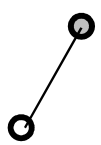
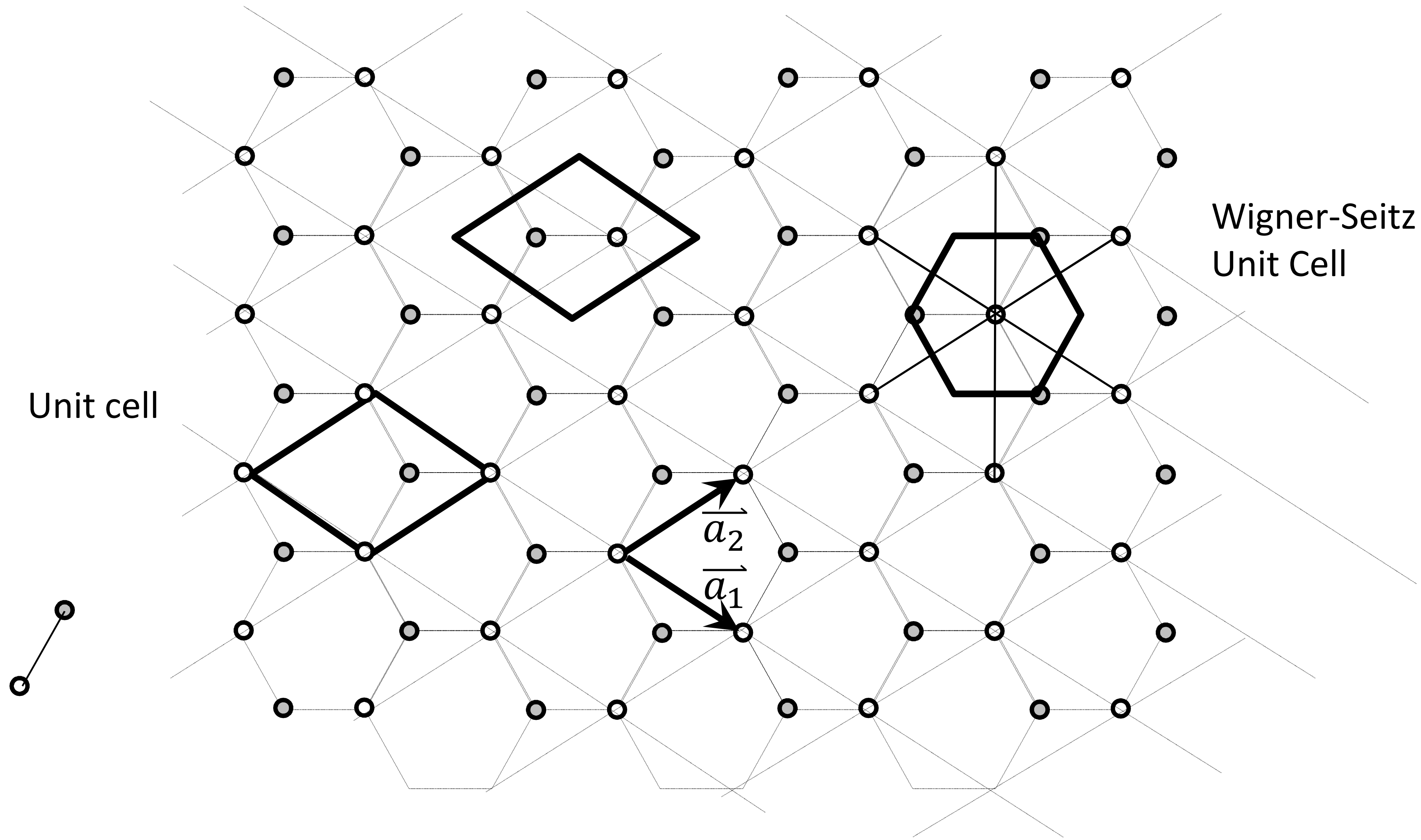




Crystal Lattice, Graphene

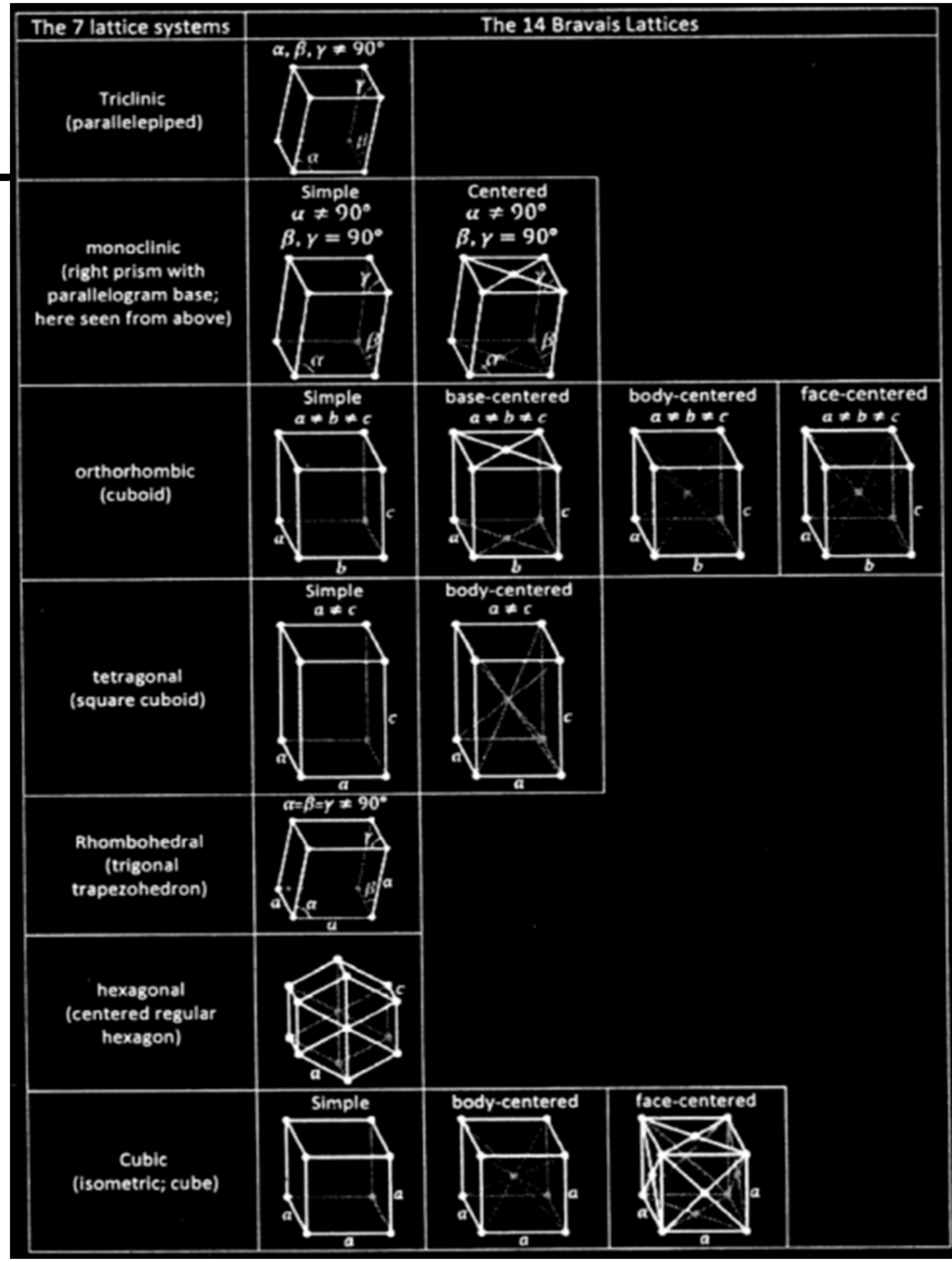
Example: Graphene

Honeycomb structure



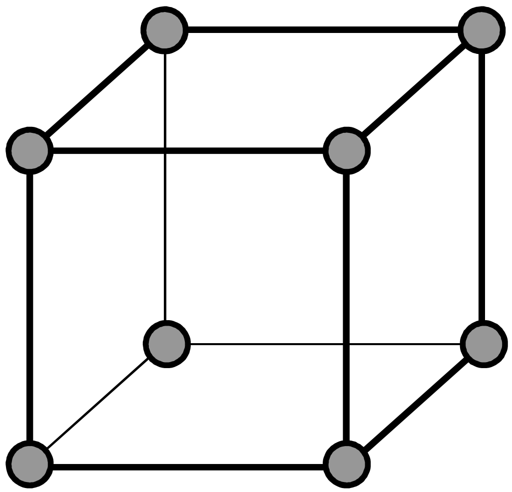
Bravais Lattices in 3D

There are 14 Bravais lattices in 3D

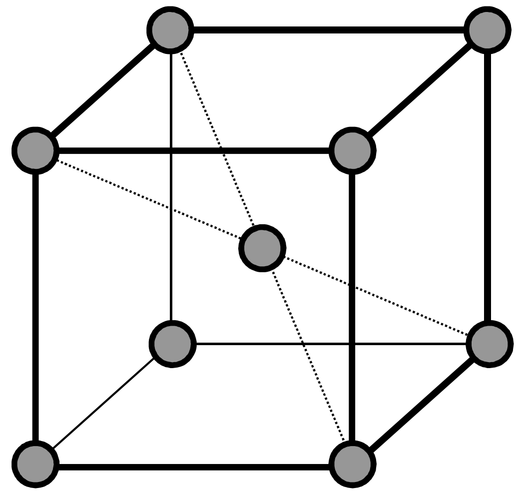


Cubic Lattices

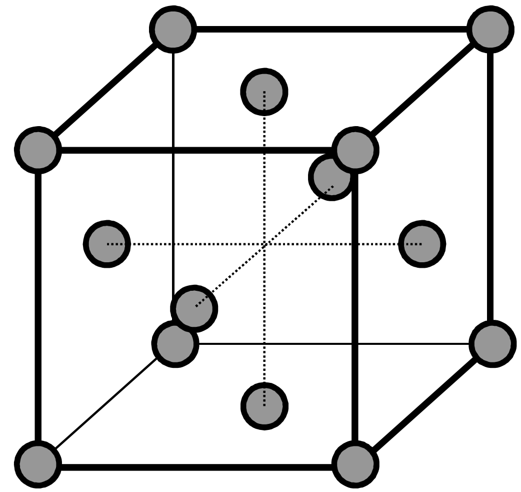
Simple cubic (SC)



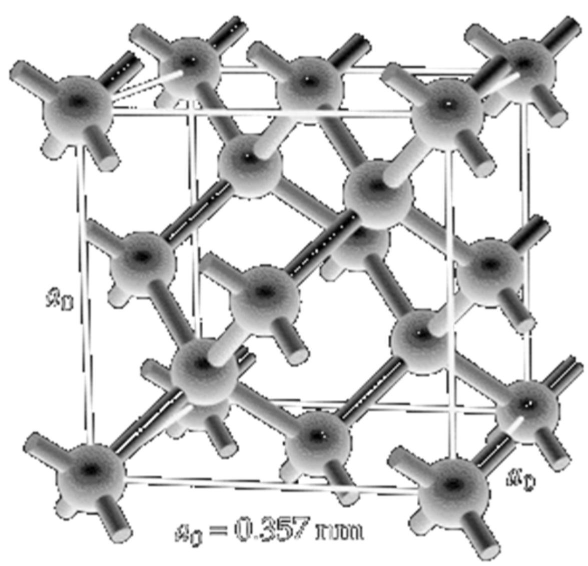
Body-centered cubic (BCC)



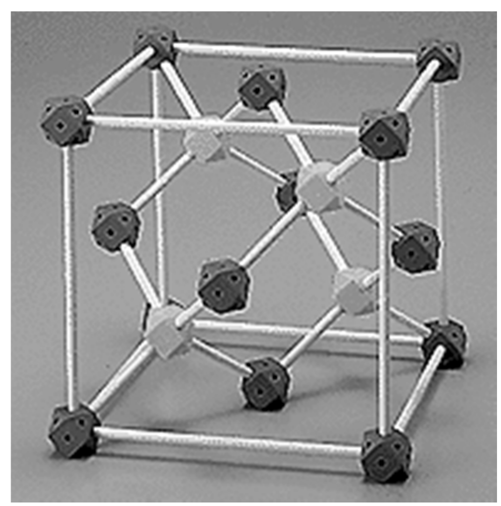
Face centered cubic (FCC)



Diamond Lattice



Zinc Blende Structure



Simple cubic (SC)

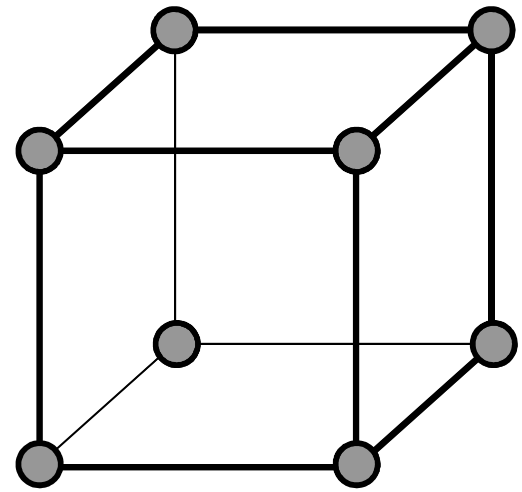
Example:

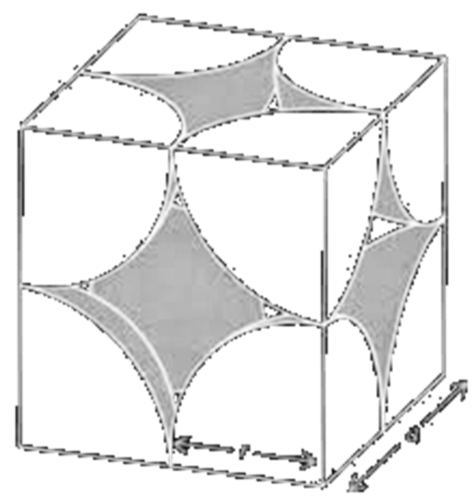
alpha polonium

Coordination Number (# of nearest nbs.) =

# of atoms/cell =

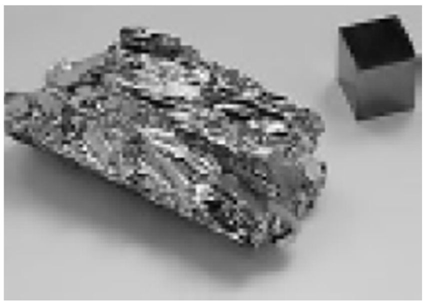
Packing fraction =

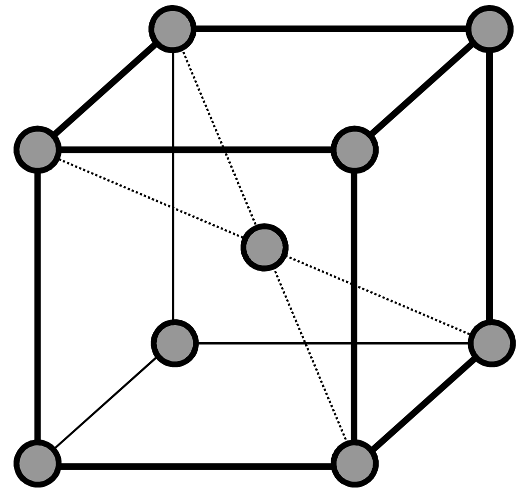




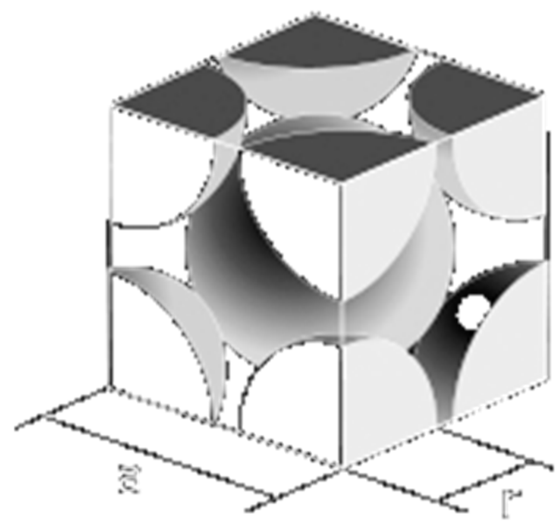
Body-centered cubic (BCC)

Example:
Sodium, Molybdenum, Tungsten



Coordination Number (# of nearest nbs.) =
# of atoms/cell =
Packing fraction =

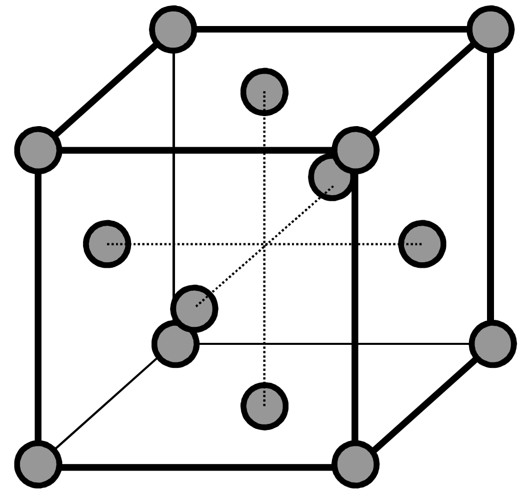


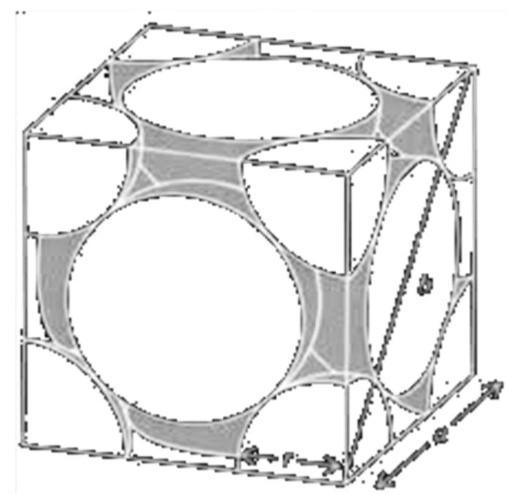
Face centered cubic (FCC)

Example:

Aluminum, Copper,

Gold, Silver,



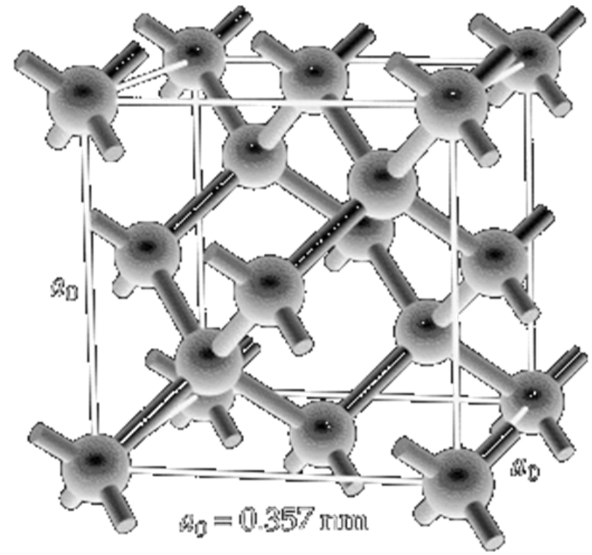


Coordination Number (# of nearest nbs.) =

# of atoms/cell =

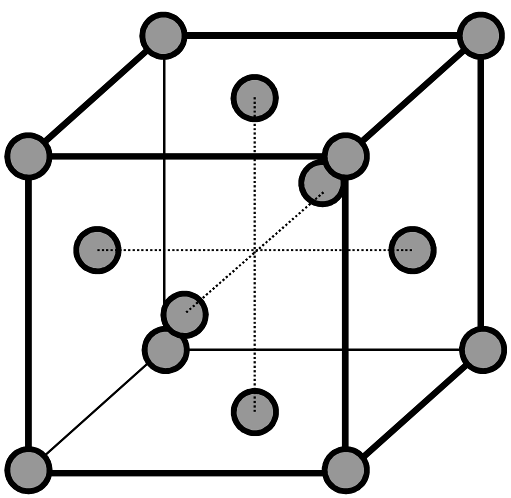
Packing fraction =

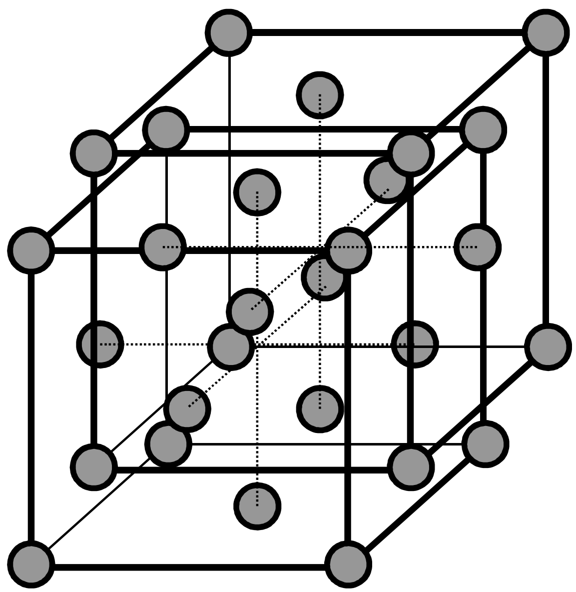
Diamond Lattice

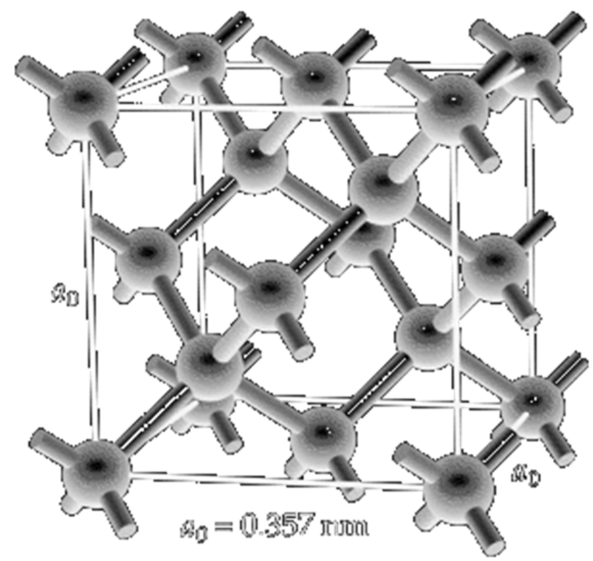


Example:
Silicon, Germanium, Carbon

Coordination Number (# of nearest nbs.) =
# of atoms/cell =
Packing fraction =







Diamond Lattice

Example:

Silicon, Germanium, Carbon

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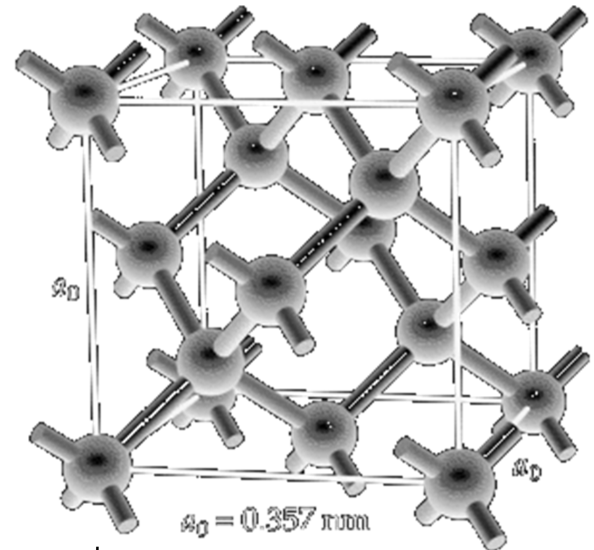


lattice constant

$= 5.431\ A$

cell volume:

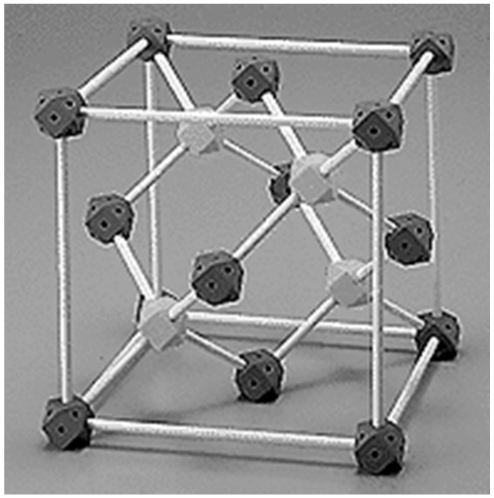
$(0.543\text{ nm})^3 = 1.6 \times 10^{-22}\text{ cm}^3$

Density of silicon atoms

$= (8\text{ atoms}) / (\text{cell volume}) = 5 \times 10^{22}\text{ atoms/cm}^3$

Zinc Blende Structure

III-V semiconductors, important for optoelectronics.



GaAs, InP,
InGaAs,
InGaAsP,........

For GaAs:
Each Ga surrounded By 4 As,
Each As Surrounded by 4 Ga

Symmetry

Many physical properties depends on the symmetry

n- fold rotational symmetry

C_n: $2\pi/n$ rotation ($n = 1,2,3,4,6$)

Inversion center symmetry

$I: r \longmapsto -r$

no center symmetry → piezoelectricity

plane of symmetry (reflection)

σ

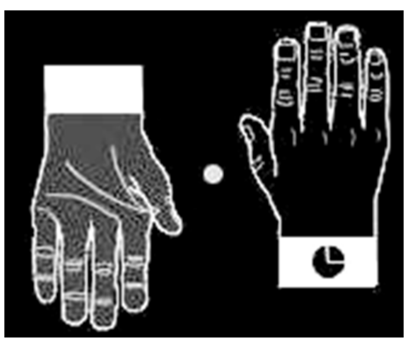
rotation – inversion symmetry

S_n: $C_n + \sigma$

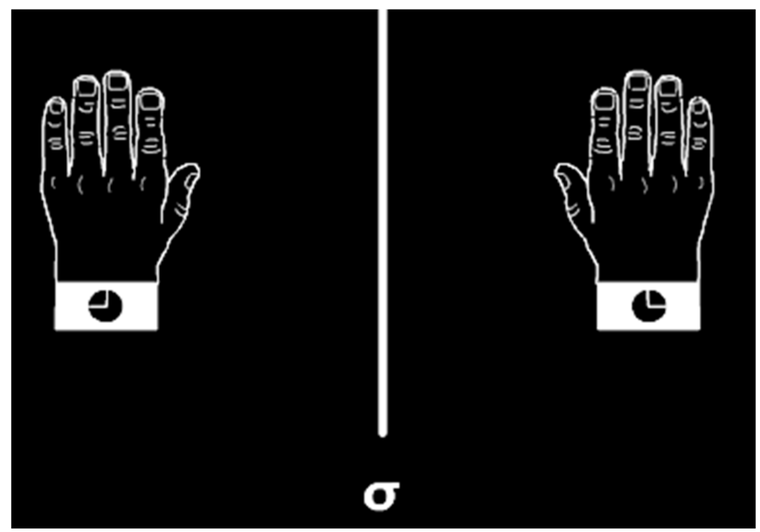
Symmetry

C_n $n = 2$ $n = 3$ $n = 10$

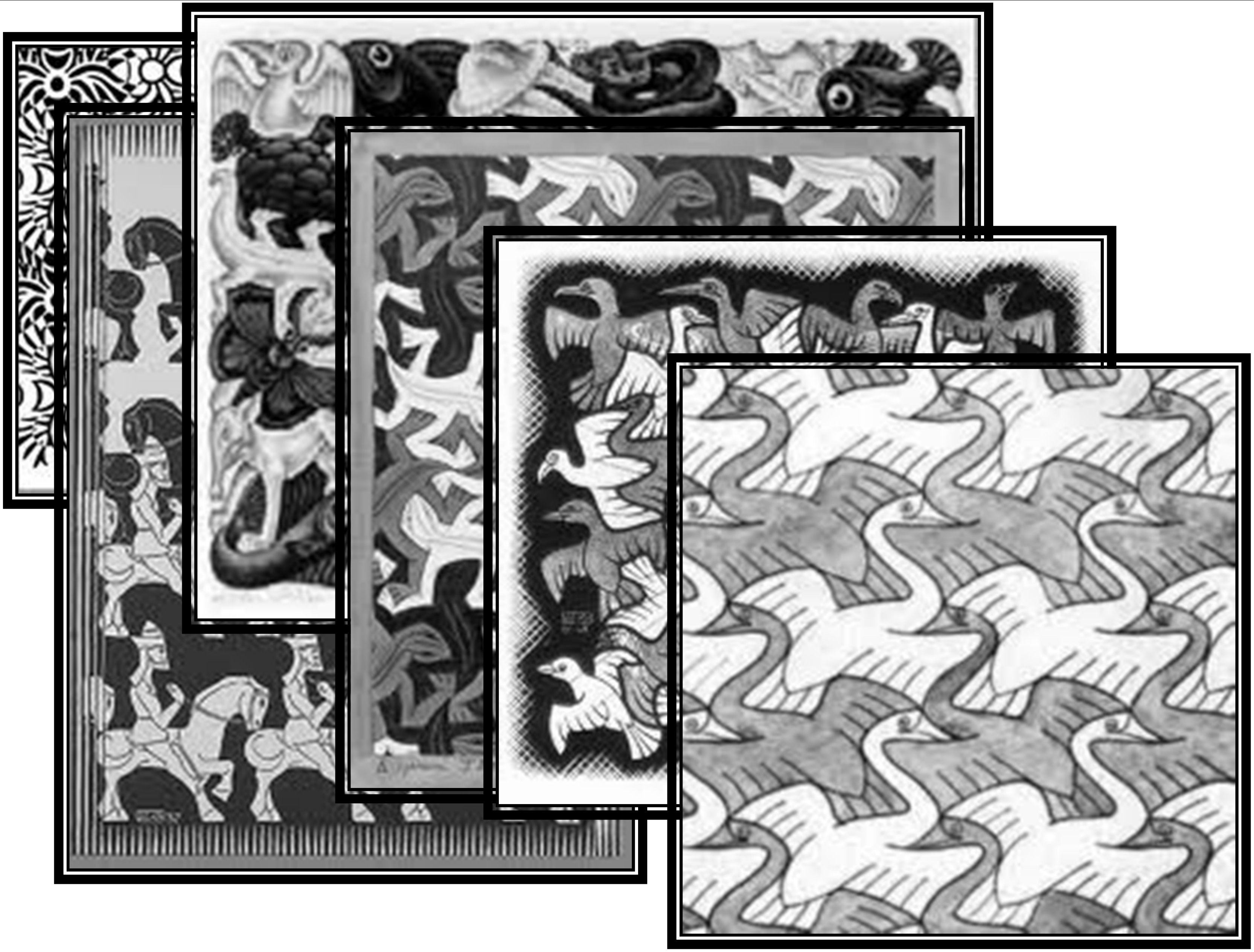
$I\colon r \longmapsto -r$



σ

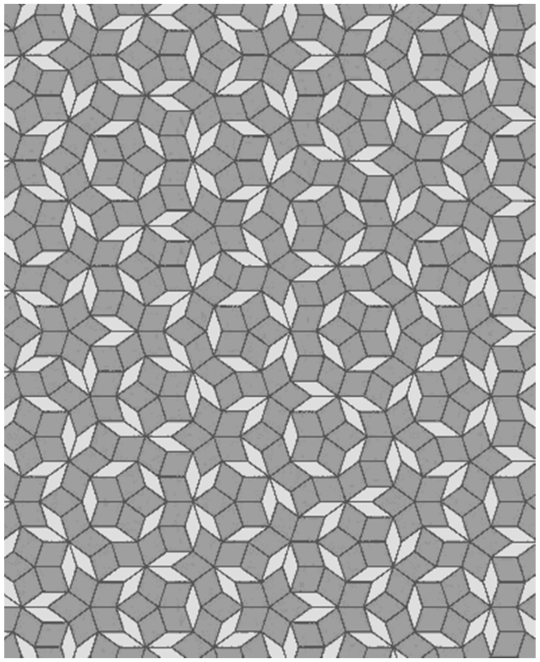


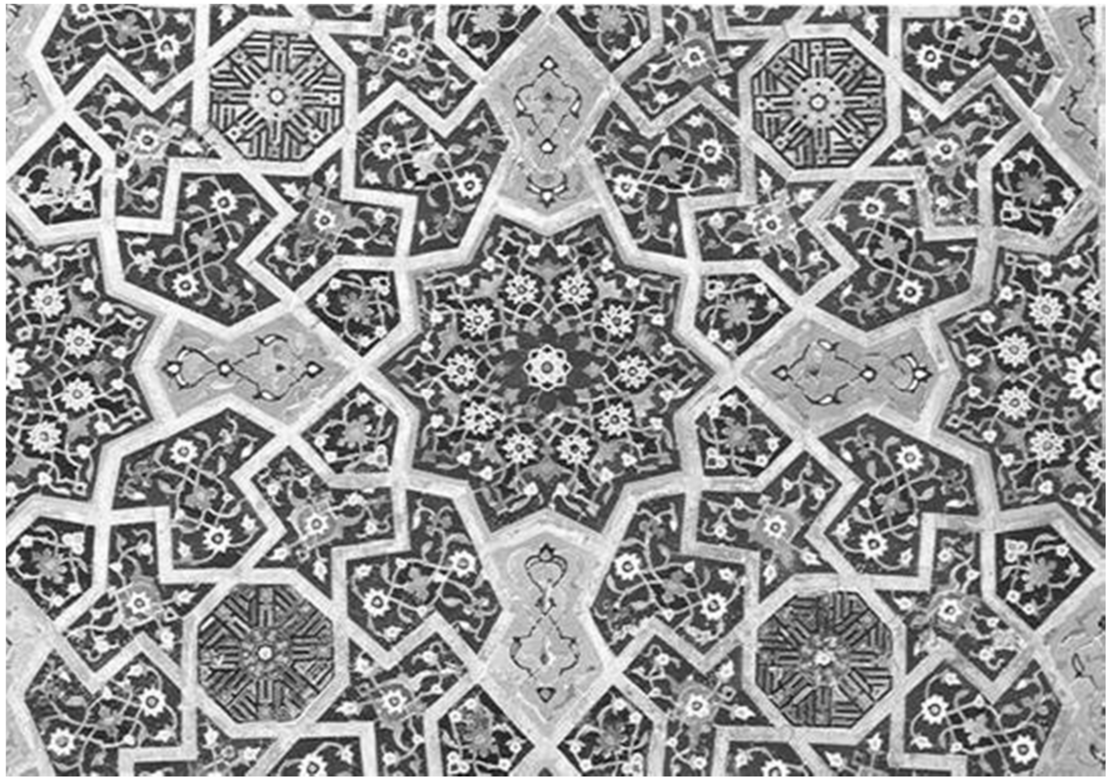
M. C. Escher

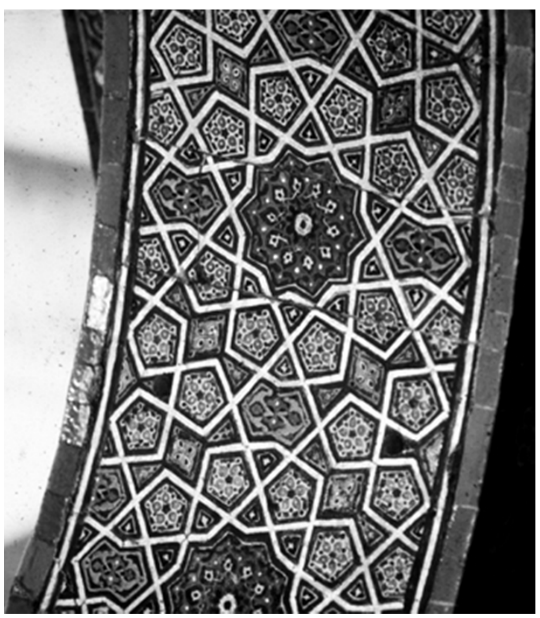


M C Escher
(1898 – 1972)

Non-Bravais Lattices







SCIENCE VOL 315 23 FEBRUARY 2007

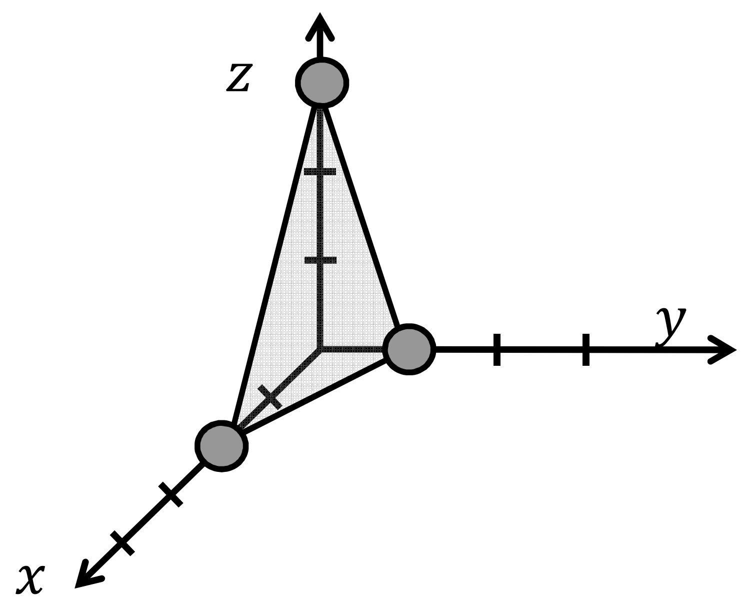
Decagonal and Quasi-Crystalline Tilings in Medieval Islamic Architecture

Peter J. Lu[1*] and Paul J. Steinhardt[2]

http://www.npr.org/templates/story/story.php?storyId=7544360
http://wwwphy.princeton.edu/~steinh/islamictilings.html

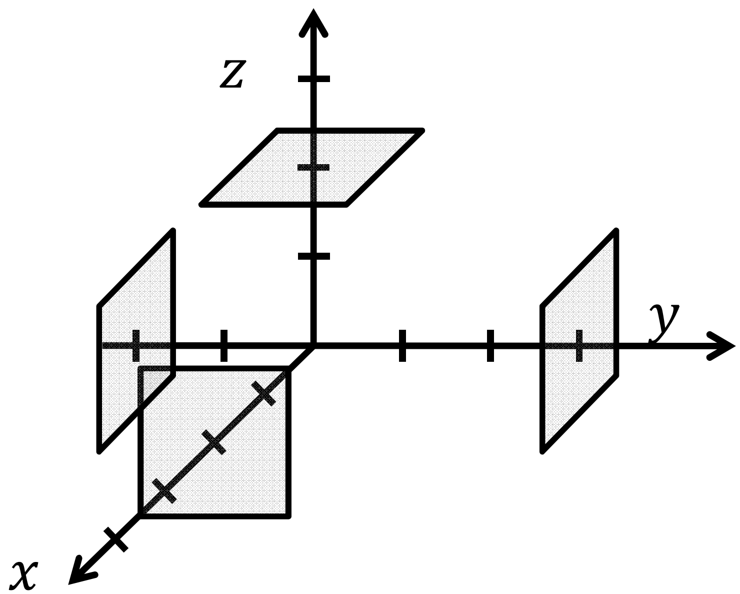
Miller Indices

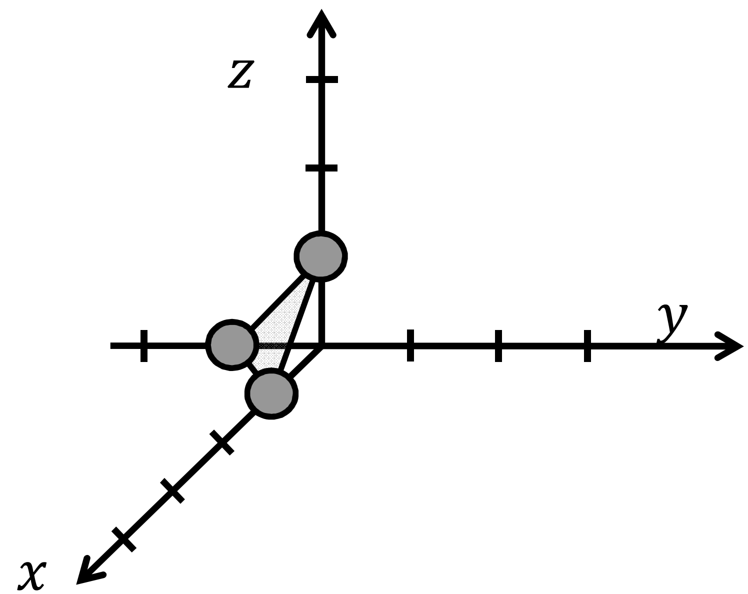
A method to label distinct planes and direction within a crystal structure.
steps:
1. Note where the plane to be indexed intercepts the axes (chosen along unit cell directions). Record result as whole numbers of unit cells in the x, y, and z directions, e.g., 2, 1, 3.
2. Take the reciprocals of these numbers, e.g., 1/2, 1, 1/3
3. Convert to whole numbers with lowest possible values by multiplying by an appropriate integer, e.g., x6 gives 3, 6, 2.
4. Enclose number in parentheses to indicate it is a crystal plane categorization, e.g., (3,6,2)



Miller Indices

Planes parallel to a unit cell coordinate axis are viewed as intercepting the axis at infinity, so have an associated Miller index in that direction of zero, e.g., (100) plane.
Planes intersecting along the negative axis use a bar over the index rather than a negative sign, e.g., $\bar{1}$ rather than -1, e.g., $(1\bar{1}1)$.
Groups of equivalent planes,($(100), (010), (001), (\bar{1}00), (0\bar{1}0)$, and $(00\bar{1})$all equivalent because rotation about the 3 fold axes on the cube diagonals maps the various faces into one another, making the planes equivalent) are notated in curly brackets, i.e., $\{100\}$ for the above set of equivalent planes.





Miller Indices

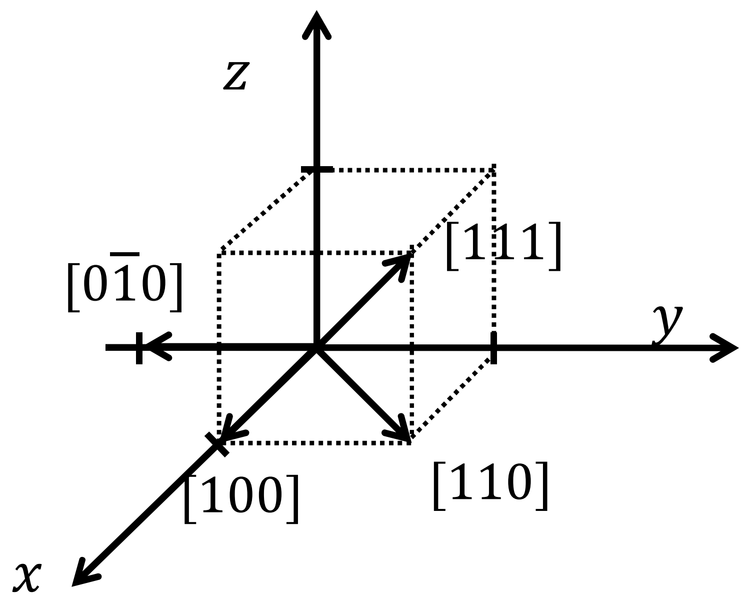
Similar procedure can be used to define Miller indices for directions.

1. Set up a vector of arbitrary length in the direction of interest (must be a crystal direction, i.e., connecting two crystal points)
2. Decompose the vector into its basis vector components in the a, b, and c directions
3. Convert the resulting numbers to the lowest possible set of integers by multiplying by an appropriate number

Directions are notated using square brackets, e.g., $[1\bar{1}1]$

For cubic crystals, directions perpendicular to particular crystal planes can be indexed using the same index as the plane. Sets of equivalent directions are specified by triangular brackets, e.g., $\langle 100 \rangle$

$$[h, k, l] \perp (h, k, l)$$

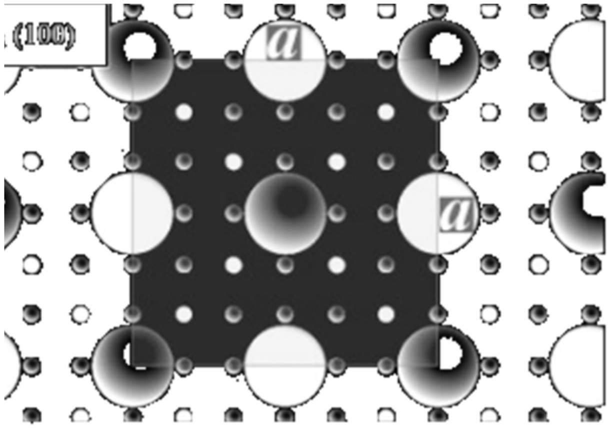


Miller Convention Summary

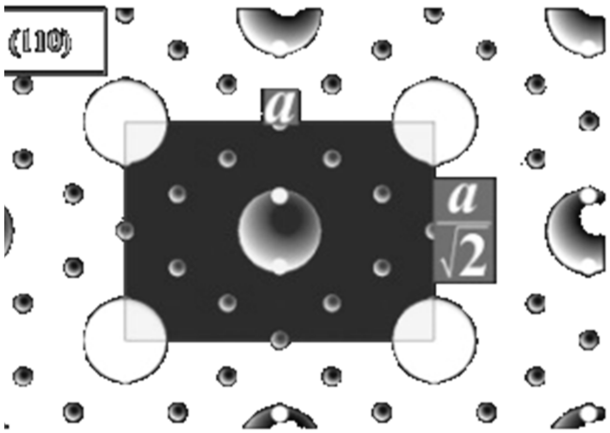
Convention	Interpretation
(hkl)	Crystal plane
$\{hkl\}$	Equivalent planes
$[hkl]$	Crystal direction
$\langle hkl\rangle$	Equivalent directions

Crystallographic Planes

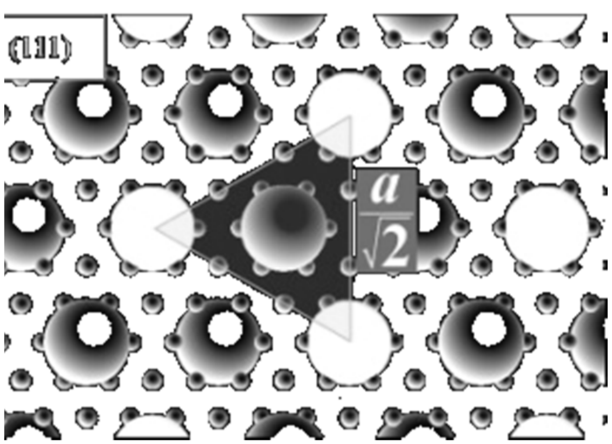
(100)



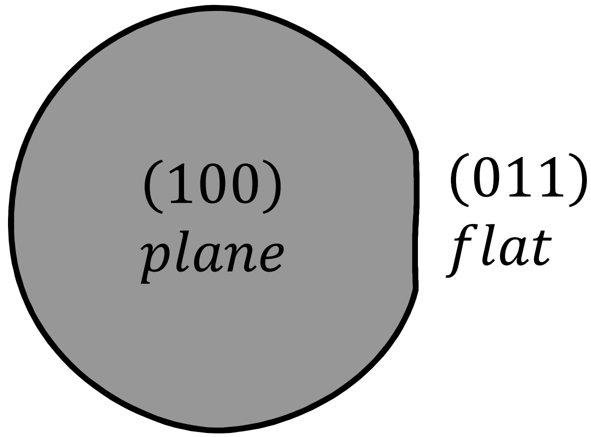
(110)

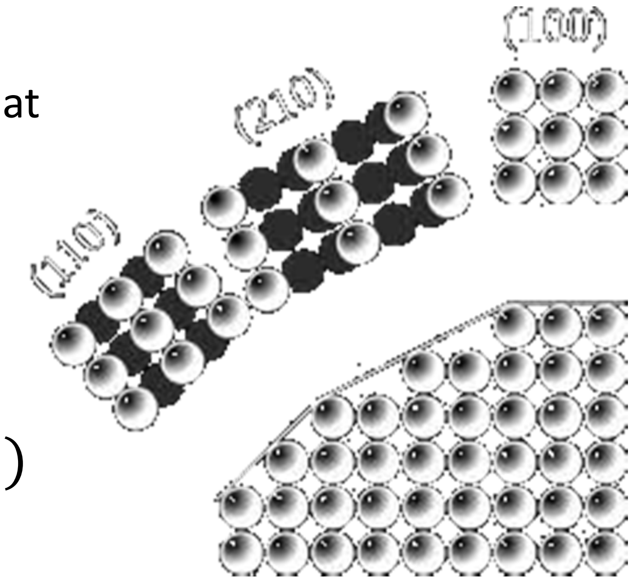


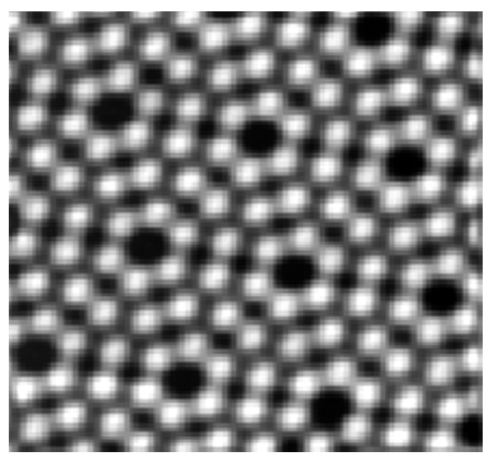
(111)



Silicon wafers are usually cut along the (100) plane with a flat or notch to help orient the wafer during IC fabrication.







(111) view