Miller Indeces

Manuel Toledo

NEL 5209 - Solid State Devices

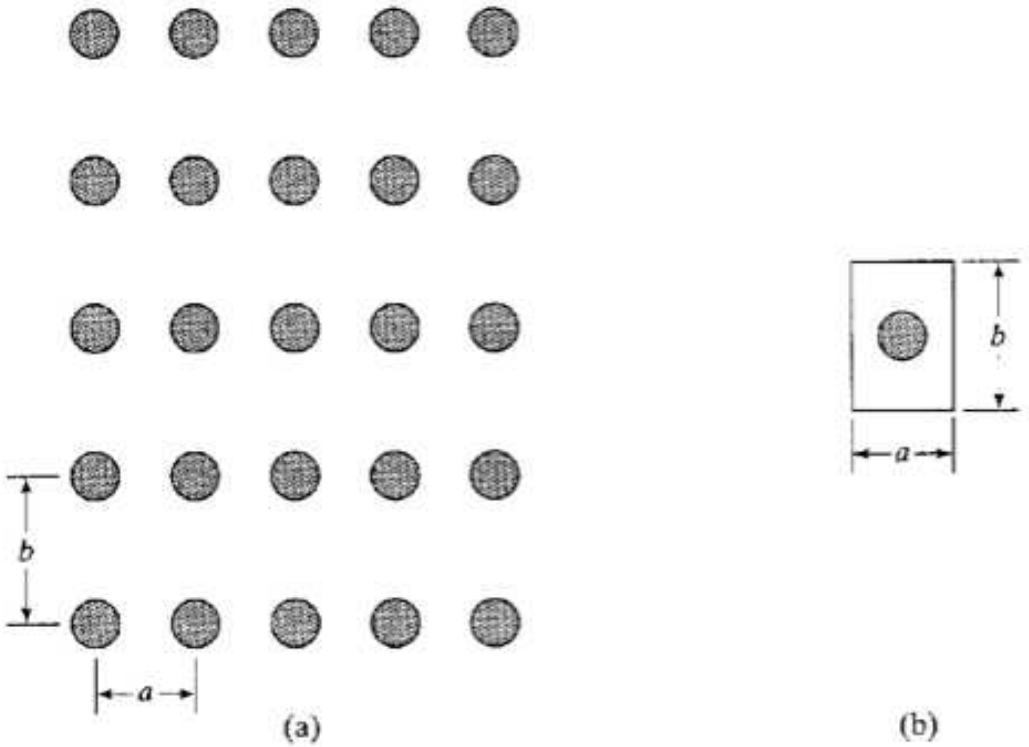
Lecture 2 - Spring 2012

mtoledo@ece.uprm.edu

Electrical and Computer Engineering

University of Puerto Rico

Review - Unit cells



(a) Sample 2D lattice and (b) unit cell.

Review - Unit cells

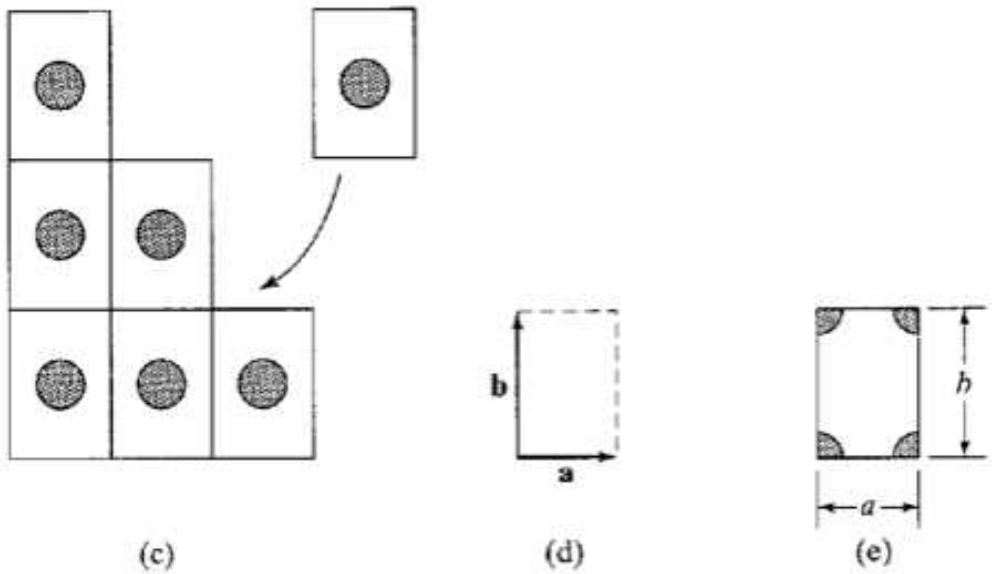


Figure 1.1 Introduction to the unit cell method of describing atom arrangements within crystals. (a) Sample two-dimensional lattice. (b) Unit cell corresponding to the part (a) lattice. (c) Reproduction of the original lattice. (d) Basis vectors. (e) An alternative unit cell.

Review - Cubic 3D cells

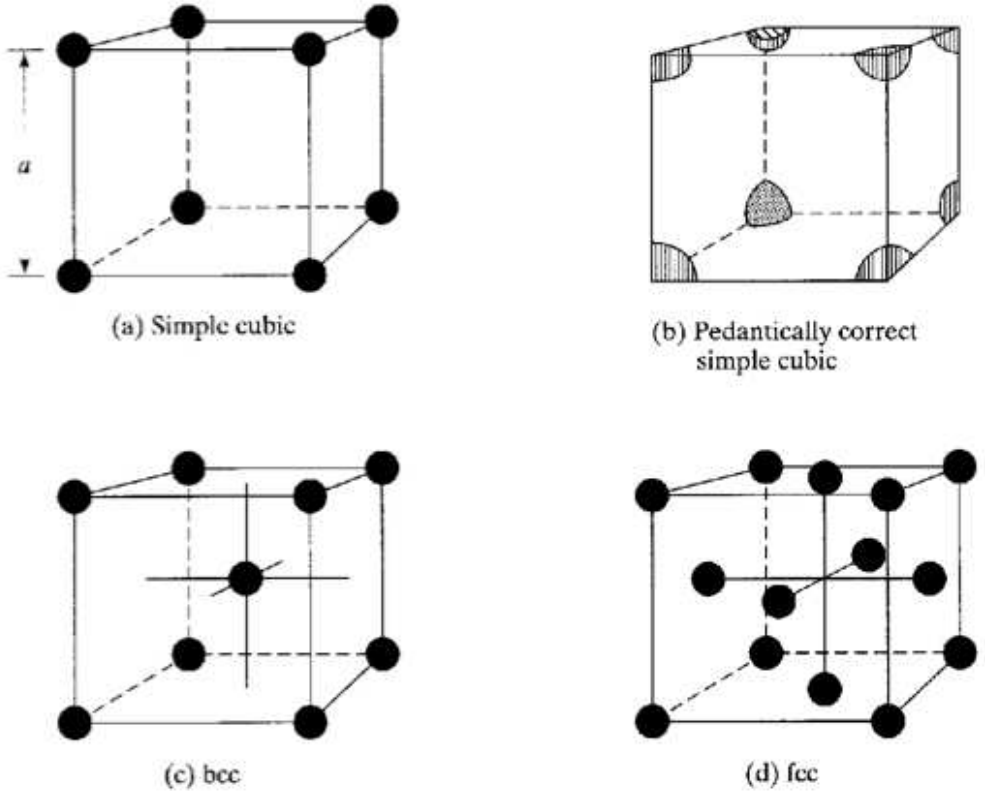
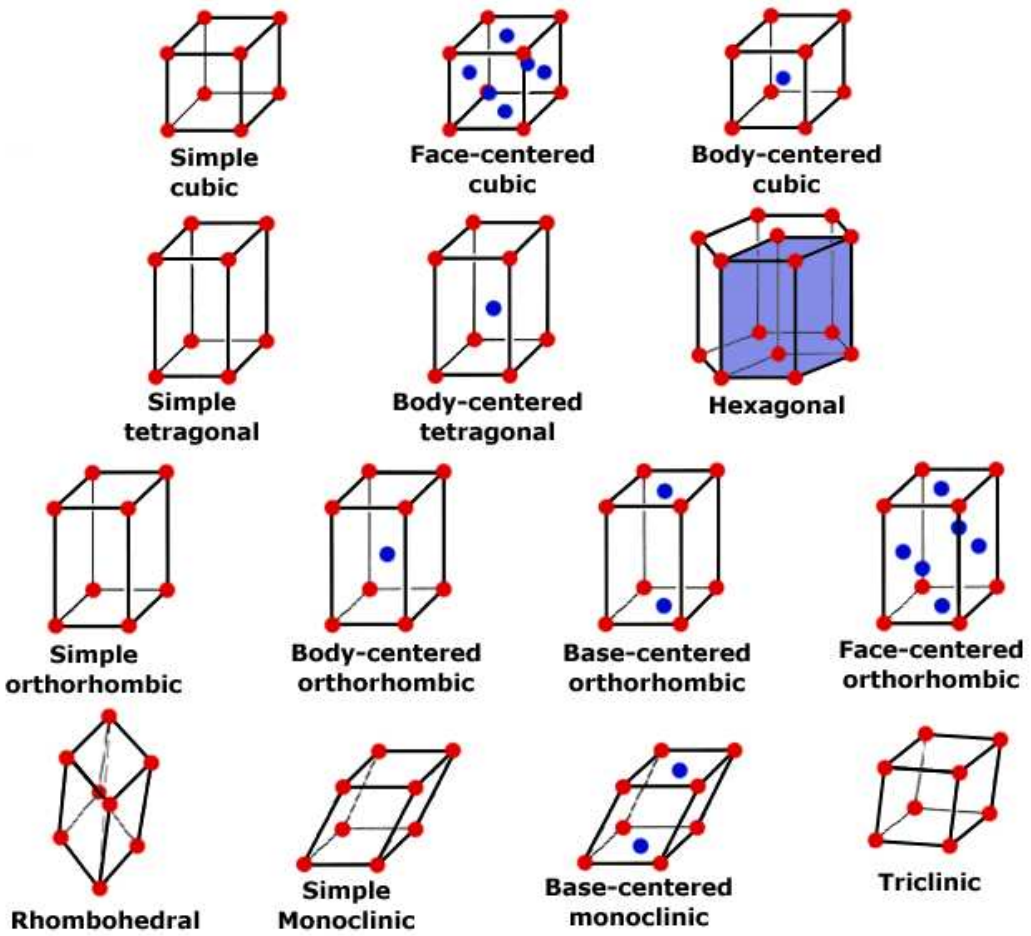


Figure 1.2 Simple three-dimensional unit cells. (a) Simple cubic unit cell. (b) Pedantically correct simple cubic unit cell including only the fractional portion (1/8) of each corner atom actually within the cell cube. (c) Body-centered cubic unit cell. (d) Face-centered cubic unit cell (After Pierret.[3])

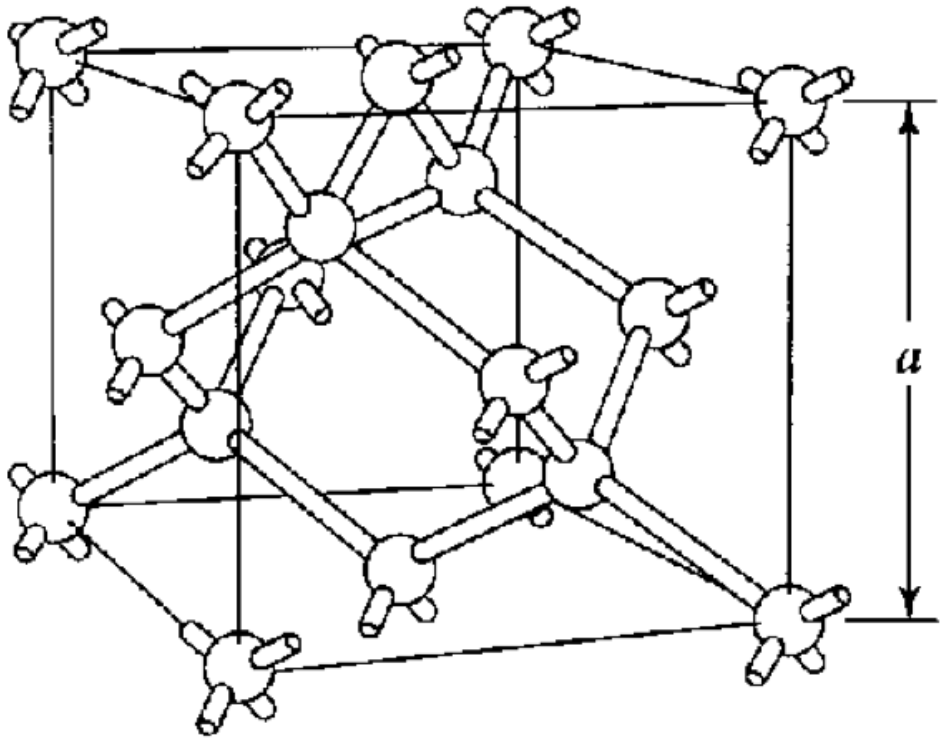
Review - Bravais lattices



Review - Unit Cells

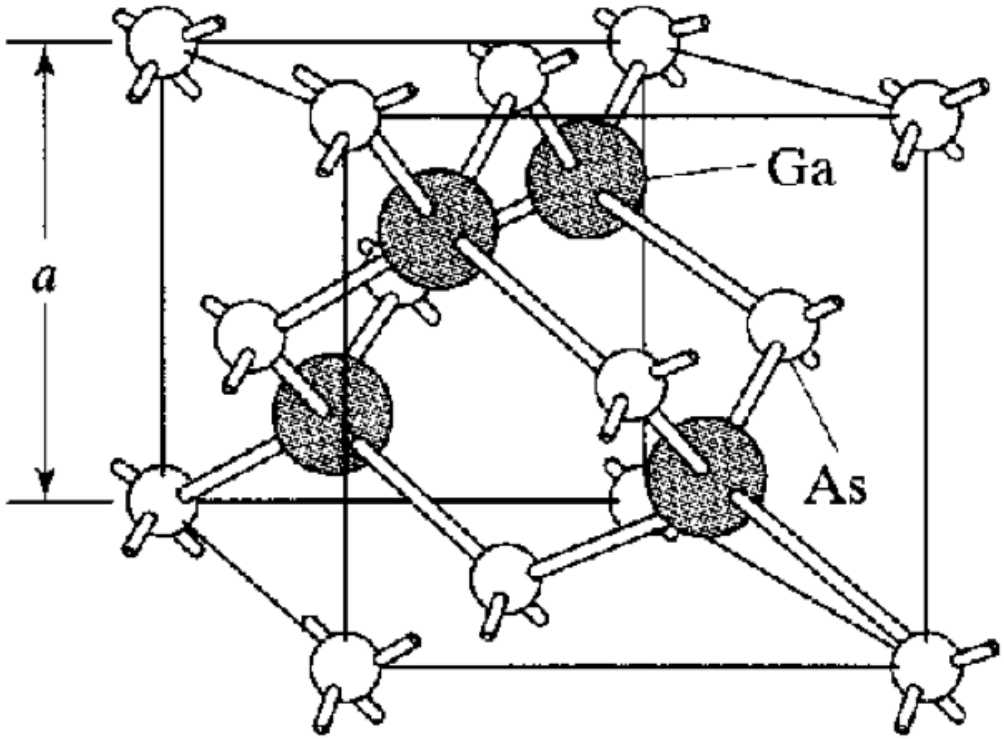
- Unit cells are not unique.
- A unit cell need not to be primitive.
- A primitive cell is the smallest unit cell possible.
- The Bravais lattices represent the 14 unique ways of arranging points in a 3D lattice.
- Lattice points do not correspond one-to-one to atoms in a crystal.

Review - Diamond unit cell



Si and Ge crystallize in the diamond unit cell.

Review - Zinc-Blende u.c.

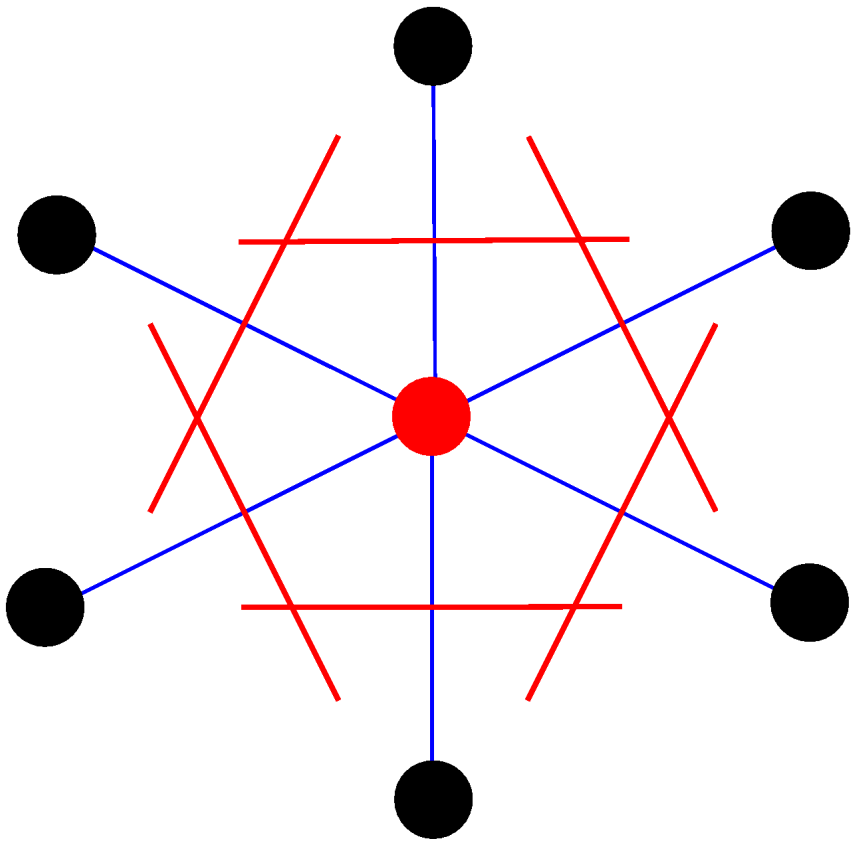


GaAs crystallizes in the Zinc-Blende unit cell.

Wigner-Seitz Unit Cell

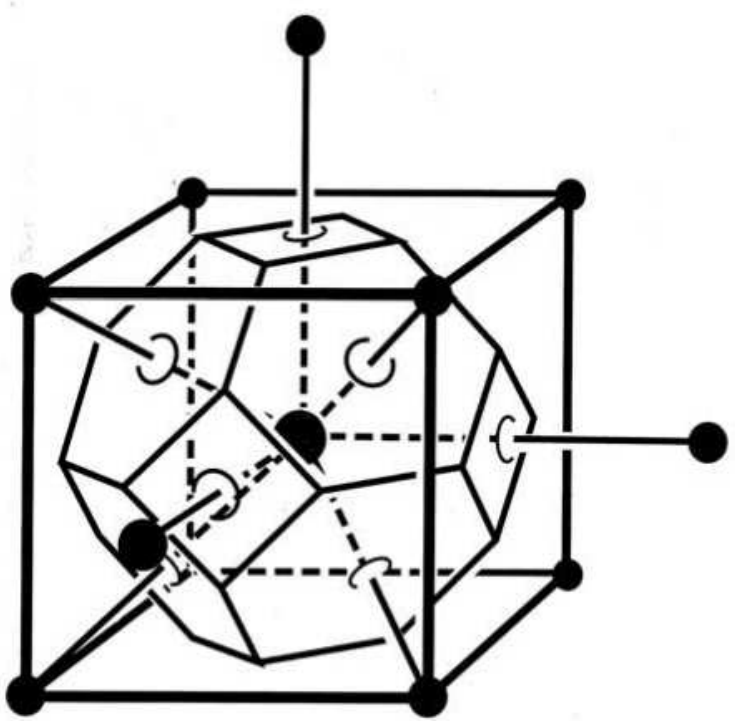
- Way of defining the u.c.
- Preserve symmetry of lattice
- Constructed a s follows:
  1. Close a lattice point as the origin
  2. Draw lines from this origin to all nearby lattice points
  3. Erect planes normal to each tie line and placed halfway between the lattice points.
  4. The planes intercept and form a 3D box.
  5. The smallest volume enclosed by this construction is the WS unit cell.

Wigner-Seitz Cell



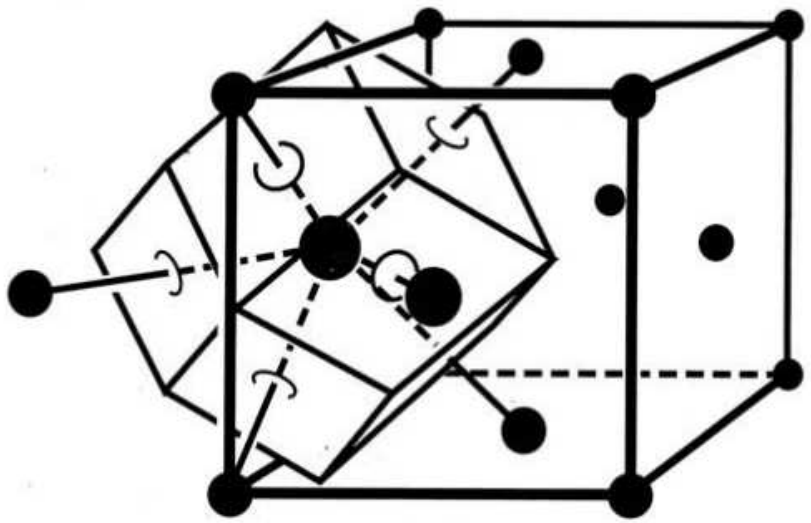
Cell construction.

W-S Cell for BCC



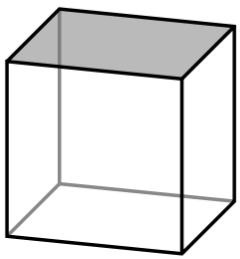
WS cell for the bcc lattice.

WS Cell for FCC

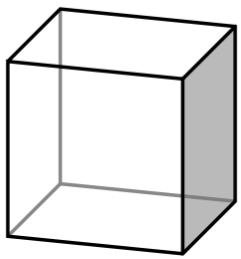


WS cell for the fcc lattice.

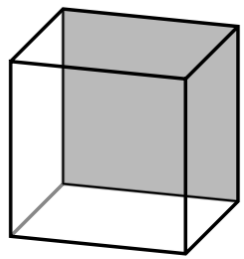
Miller indeces



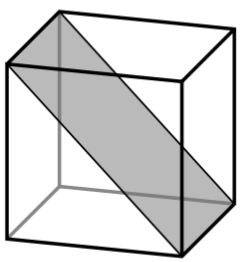
(001)



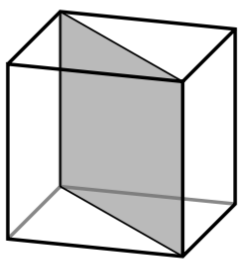
(100)



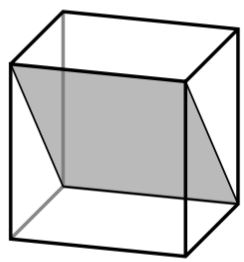
(010)



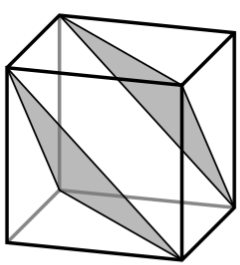
(101)



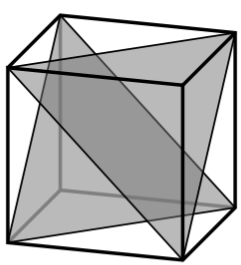
(110)



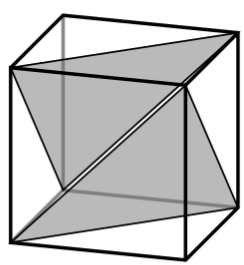
(011)



(111)

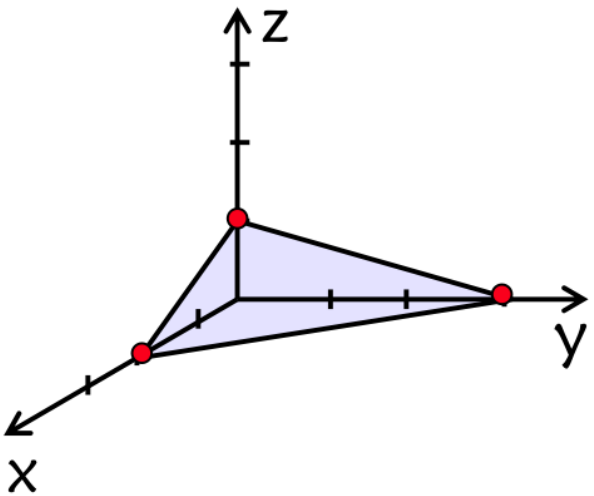


$(1\bar{1}1)$



$(\bar{1}11)$

Miller indices for planes



- set axes along the edges of the unit cell
- find normalized intercepts: $2, 3, 1$
- invert: $1/2, 1/3, 1$
- common numerator: $3/6, 2/6, 6/6$
- miller indices are (326)

Miller indices for planes

Example 2

- intercept is: $2, 1, -2$
- reciprocals: $1/2, 1, -1/2$
- express as: $1/2, 2/2, -1/2$
- indices: $(12\bar{1})$

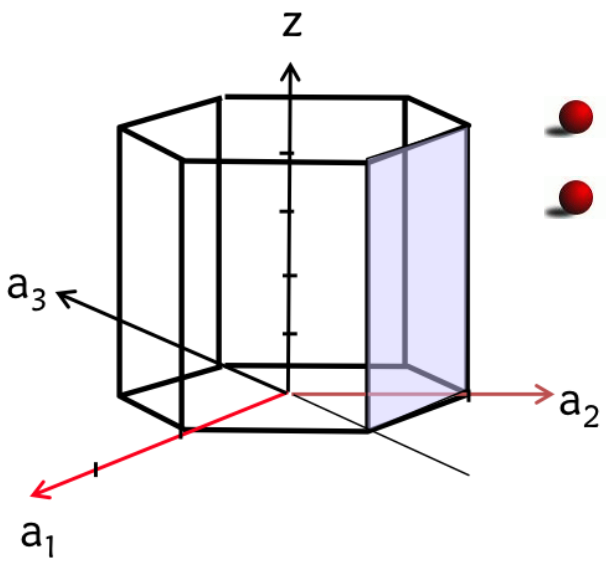
Miller indices for planes

Example 3

- Plane is parallel to z-axis
- Intercepts: $2, 3, \infty$
- Reciprocals: $1/2, 1/3, 0$
- Indices: (320)

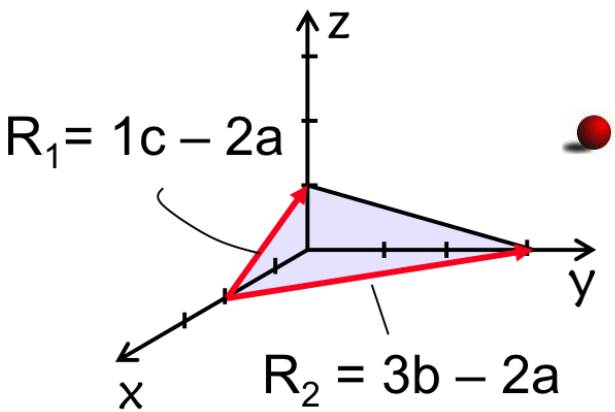
Bravais-Miller Indices

Used for Hexagonal lattices.



- Use four axes:
  - $a_{1,2,3}$ on the base, 120° from each other
  - the other (Z) perpendicular to $a_{1,2,3}$
- Consider the surface parallel to a_1 and to Z
- 4 indexes:
  - Intercepts: $\infty, 1, -1, \infty$
  - Indices: $(01\bar{1}0$

Miller indices



a,b, c: unit vectors in x, y and c axes

- $\vec{R_1} = 1c - 2a$
- $\vec{R_2} = 3b - 2a$
- $\vec{R_1} \times \vec{R_2} = \begin{vmatrix} a & b & c \\ -2 & 3 & 0 \\ -2 & 0 & 1 \end{vmatrix}$
- $\vec{R_1} \times \vec{R_2} = 3a + 2b + 6c$

Compare to slide 14.

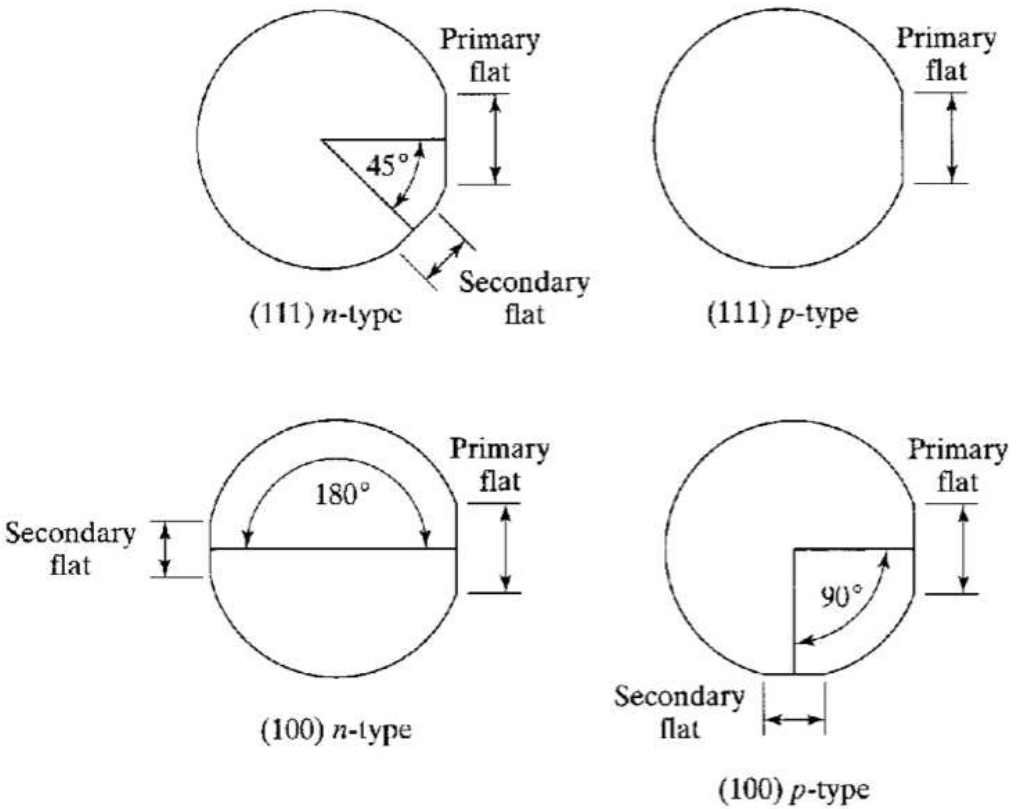
Direction: $[326]$; plane: (326)

Angle between planes

To get the angle θ between 2 planes

- $\vec{v_1}$ and $\vec{v_2}$: normalized perpendicular vectors
- $\cos\theta = \vec{v_1} \cdot \vec{v_2}$

Wafers



Textbook fig. 1.10

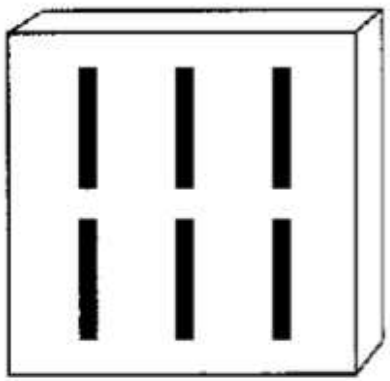
Wafers

- wafers up to 6 inches in diameter have a flat
- flat indicate type and orientation:

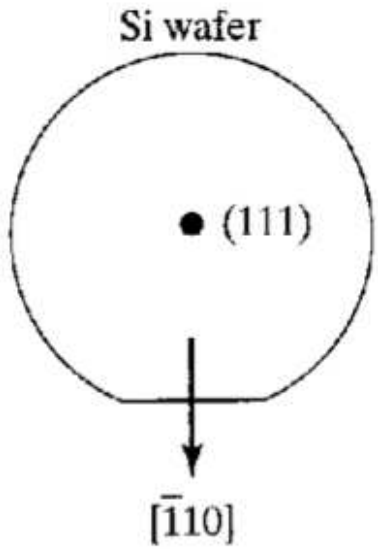
surface plane	primary flat
(100)	(011)
(111)	$(\bar{1}10)$

- bigger wafers have a small notch instead of a flat

Example



(a)



(b)

How do you position the wafer so that the pattern is aligned in the $[11\bar{2}]$ direction?