

EE 3106

Lecture 1

Introduction to Semiconductor Materials and Crystal Structures

This lecture note can be downloaded from
<http://www.ieong.net/ee3106/>

The Road Ahead

- General material properties.
- Structure of solids:
 - Amorphous, polycrystalline, crystalline.
- Crystalline solids:
 - Unit cells.
 - Lattices.
- Miller indices.
- Crystal growth.

General Material Properties

- Semiconductor is the class of material where the conductivity of the material can be controlled to vary a large orders of magnitude.

- Elemental semiconductor: Si, Ge

- Compound semiconductor (fixed composition): SiC, GaN, GaAs, InP

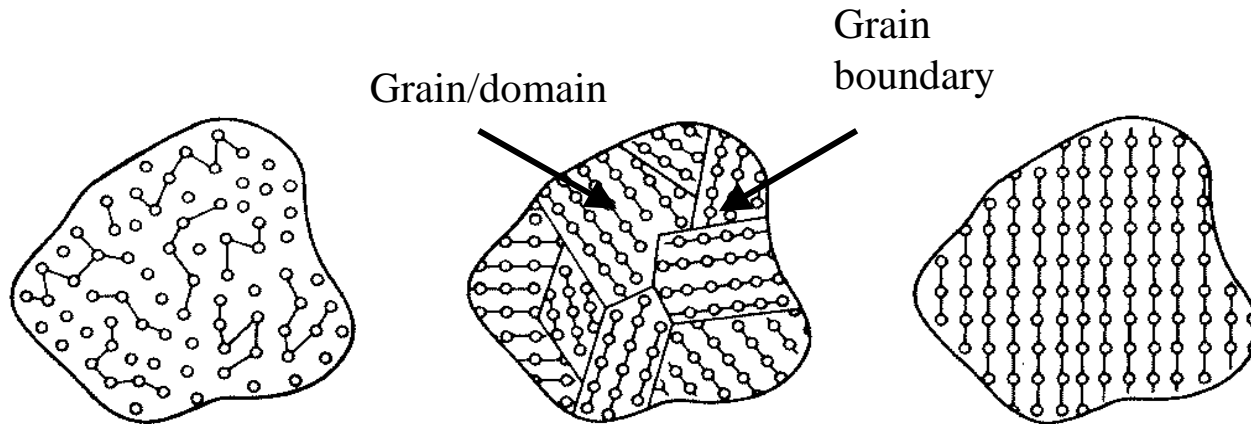
- Alloy: $\text{Si}_{1-x}\text{Ge}_x$, $\text{Al}_{1-x}\text{Ga}_x\text{As}$, $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$

- Purity:** semiconductor devices are made of semiconductors with ultra purity: unintentional doping $< 10^{-9}$ in composition, which is 0.001 ppm in solids.

- To increase range of control in conductivity (lower leakage current)

- To increase mobility (faster and more powerful devices)

Structure of solids



Amorphous

No recognizable
long-range order

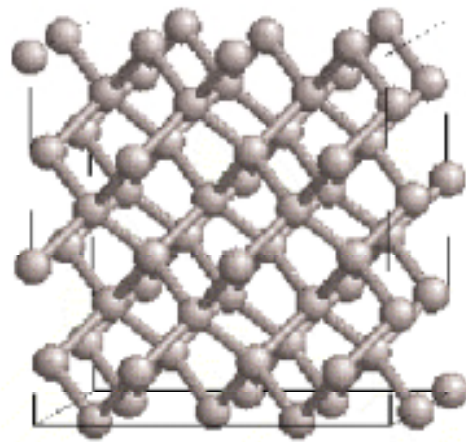
Polycrystalline

Completely ordered
In segments

Crystal

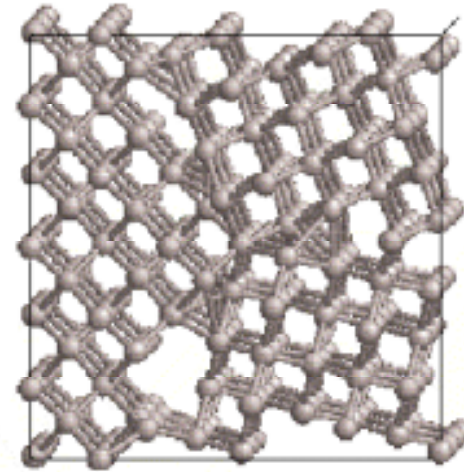
Entire solid is made
up of atoms in an
orderly array

Structure of Solids (3D View)



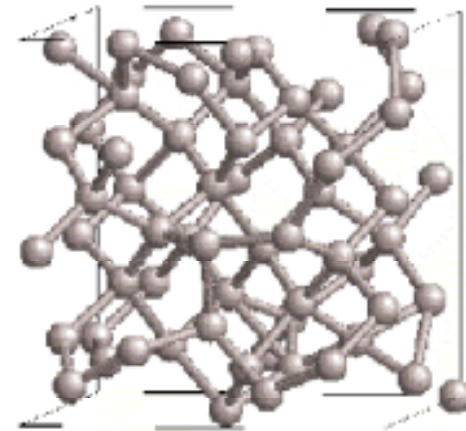
Single Crystal

All atoms arranged
on a common lattice



Polycrystalline

Different lattice orientation
for each grain

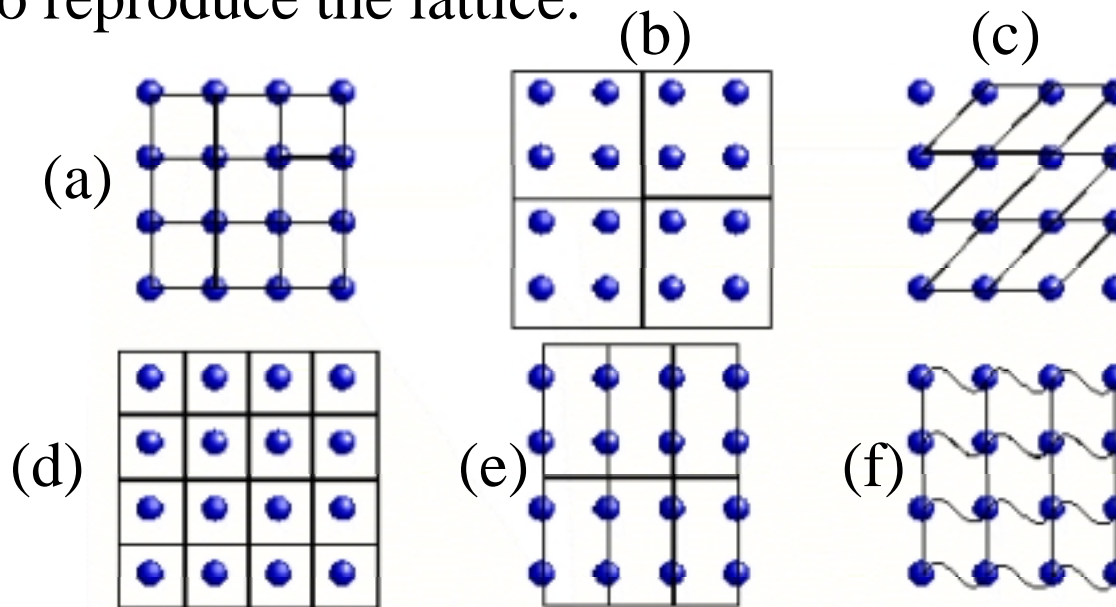


Amorphous

Atoms are disordered
(no lattice)

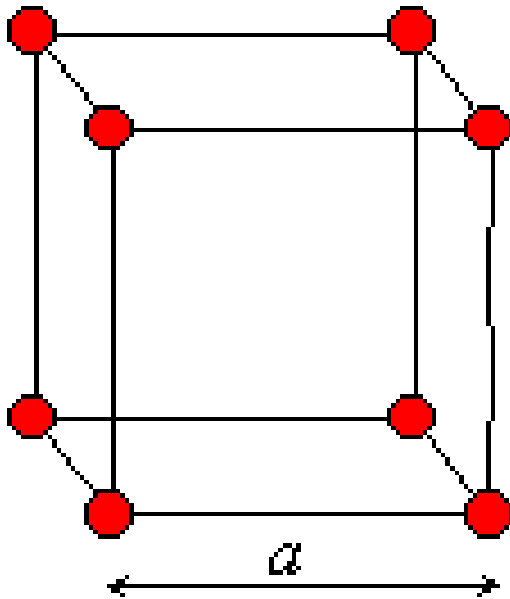
Unit Cell

➤ Unit cell is any volume that can be copied and stacked to reproduce the lattice.



- What is a primitive cell?
- Which of the above is a primitive cell?

Simple Cubic Lattice

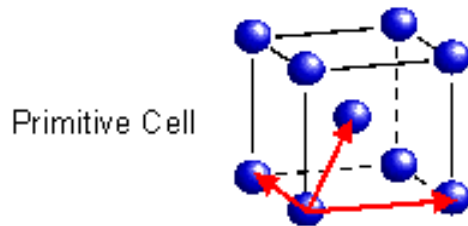
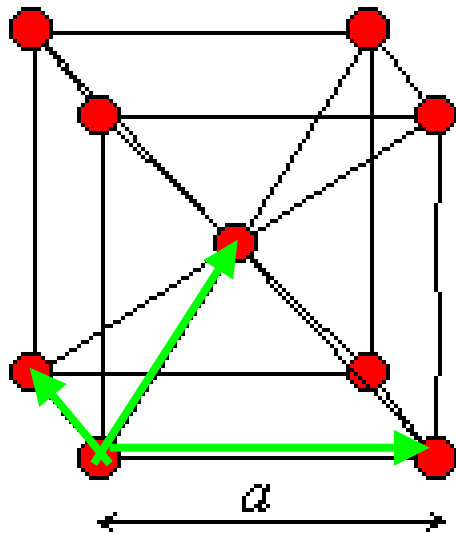


e.g.: Polonium.

Atoms per cell	$8 \times (1/8) = 1$
No. of nearest neighbors	6
Nearest neighbor distance	a
No. of 2nd nearest neighbors	12
2nd nearest neighbor distance	$\sqrt{2} a$

Body Centered Cubic (BCC) Lattice

Fill-in the table below

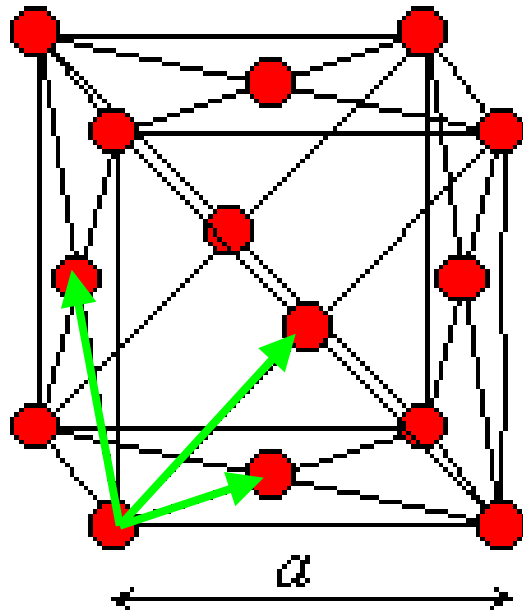


Atoms per cell	
No. of nearest neighbors	
Nearest neighbor distance	
No. of 2nd nearest neighbors	
2nd nearest neighbor distance	

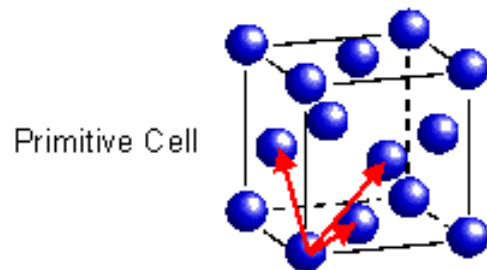
Elements with BCC lattice: Cr, Fe, K, Li, Mo, Na, Ta, and W.

Face Centered Cubic (FCC) Lattice

Fill-in the table below



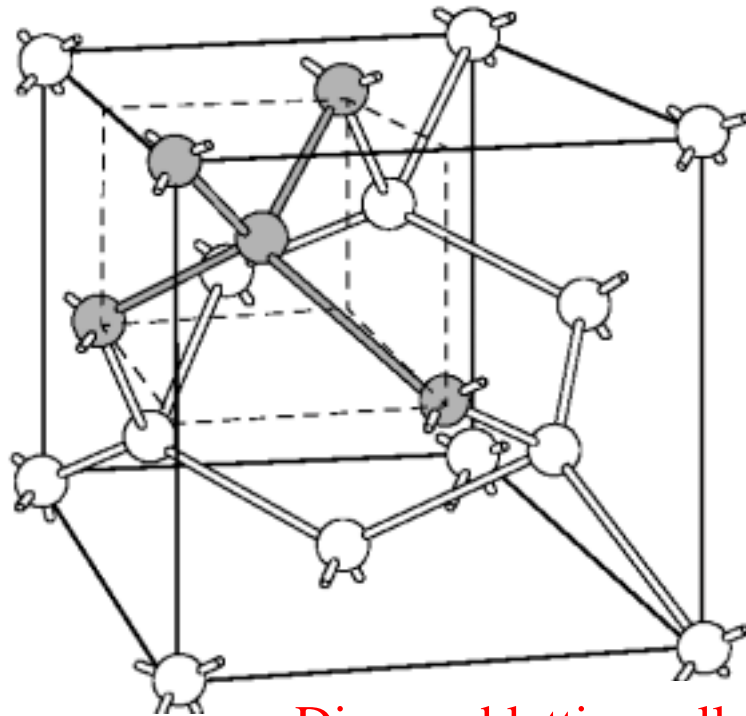
Atoms per cell	
No. of nearest neighbors	
Nearest neighbor distance	
No. of 2nd nearest neighbors	
2nd nearest neighbor distance	



Elements with FCC lattice: Al, Ag, Ca, Cu, Ni, Pb, and Pt.

Diamond Lattice

- Two interleaving FCC cells offset by $1/4$ of the cube diagonal form the lattice.
- Atoms in diamond lattice have four nearest neighbors (covalent bonds).



Diamond lattice cell
(C, Si, Ge, etc.)

Silicon Lattice Cell

Crystal Viewer - Microsoft Internet Explorer

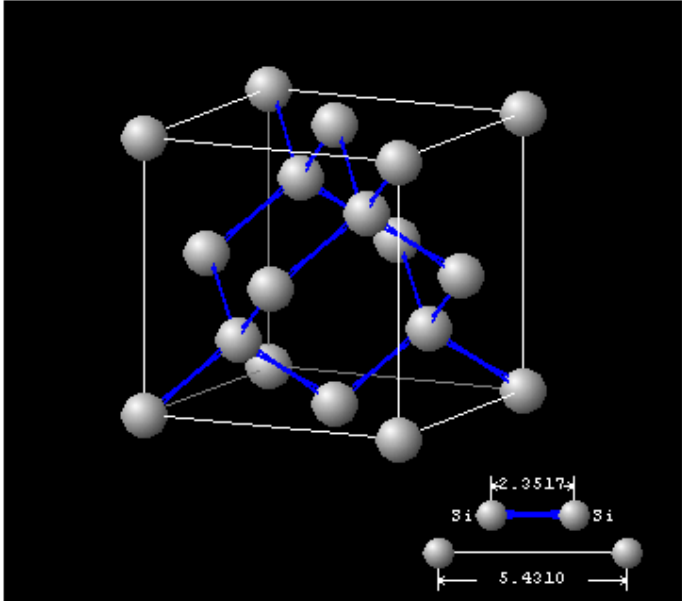
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Hide Bonds You are viewing Si unit cell. Si



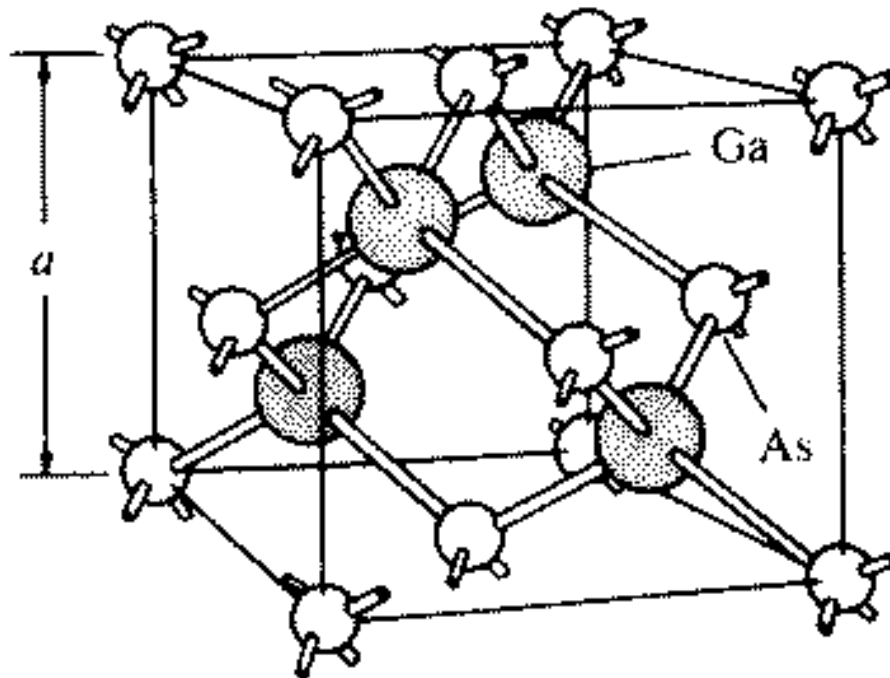
Atoms/cms	5.0E22
Atomic Weight	28.09
Breakdown field (V/cm)	~3E5
Crystal structure	Diamond
ensity (g/cm ³)	2.328
Dielectric Constant	11.9
Nc (cm ⁻³)	2.8E19
Nv (cm ⁻³)	1.04E19
Effective Mass, m*/m0	
Electrons	
m*1	0.98
m*1	0.19
Holes	
m*eh	0.16
m*hh	0.49
Electron affinity, x(V)	4.05
Energy gap (eV) at 300K	1.12
Intrinsic carrier conc. (cm ⁻³)	1.45E10
Intrinsic Debye Length (um)	24
Intrinsic resistivity (-cm)	2.3E5
Lattice constant (Å)	5.43095
Linear coefficient of thermal expansion, L/LT(C-1)	2.6E-6

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Zincblende Lattice

- Similar to diamond lattice, except that the lattice contains two different type of atoms.
- Each atom has four covalent bonds, but bonds with atoms of the other type.



Zincblende lattice cell
(GaAs, InP, AlAs, GaP, ZnS, etc.)

GaAs Lattice Cell

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Hide Bonds You are viewing GaAs unit cell. GaAs

Properties of GaAs

Atoms/cm ³	4.42E22
Atomic Weight	144.63
Breakdown field (V/cm)	~4E5
Crystal structure	Zincblende
Density (g/cm ³)	5.32
Dielectric Constant	13.1
N _c (cm ⁻³)	4.7E17
N _v (cm ⁻³)	7.0E18
Effective Mass, m*/m ₀	
Electrons	0.067
Holes	
m* _{lh}	0.08
m* _{hh}	0.45
Electron affinity, χ (V)	4.07
Energy gap (eV) at 300K	1.424
Intrinsic carrier conc. (cm ⁻³)	1.79E6
Intrinsic Debye length (μm)	2250

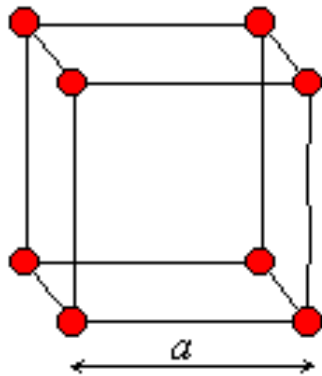
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Packing Density

Assume that the atoms are closely packed and that they can be treated as hard spheres. What is the packing density for Simple cubic?

$$\frac{\text{Volume of atoms}}{\text{Volume of the unit cell}} = \frac{\frac{4}{3} \pi r^3}{a^3} = \frac{\frac{4}{3} \pi \left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 52\%$$



	Radius	Atoms/ unit cell	Packing density
Simple cubic	$\frac{a}{2}$	1	$\frac{\pi}{6} = 52\%$
Body centered cubic	$\frac{\sqrt{3}a}{4}$	2	$\frac{\pi\sqrt{3}}{8} = 68\%$
Face centered cubic	$\frac{\sqrt{2}a}{4}$	4	$\frac{\pi\sqrt{2}}{6} = 74\%$
Diamond	$\frac{\sqrt{3}a}{8}$	8	$\frac{\pi\sqrt{3}}{16} = 34\%$

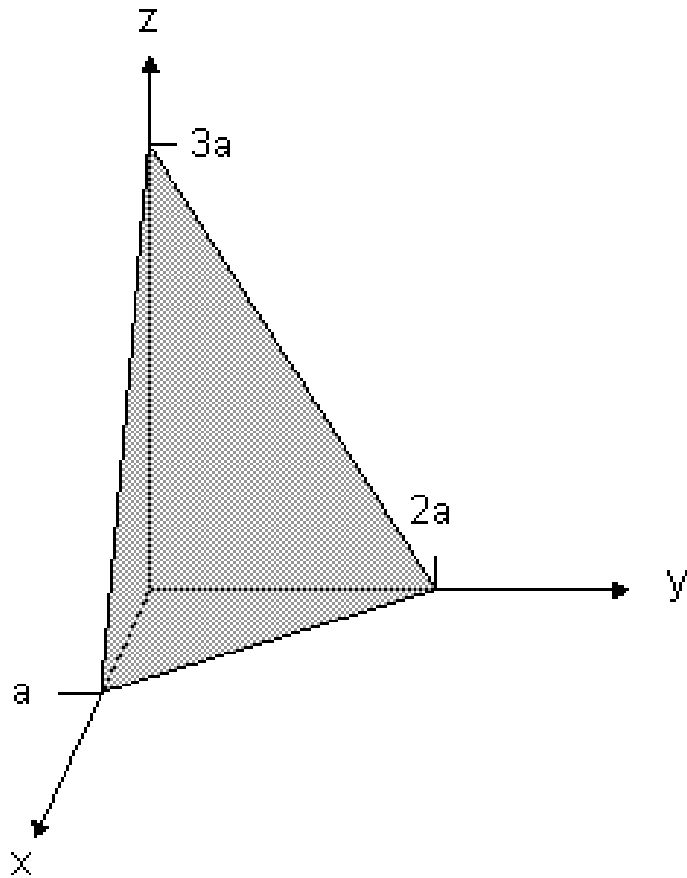
Miller Indices

- Crystal orientation is important in semiconductor processing.
- Certain device properties can depend on the orientation of the crystal lattice.
- Certain processing techniques must consider the orientation of the crystal lattice.
- Miller indices provide a conventional method to specify planes and directions in a crystal.

Miller Indices of a plane

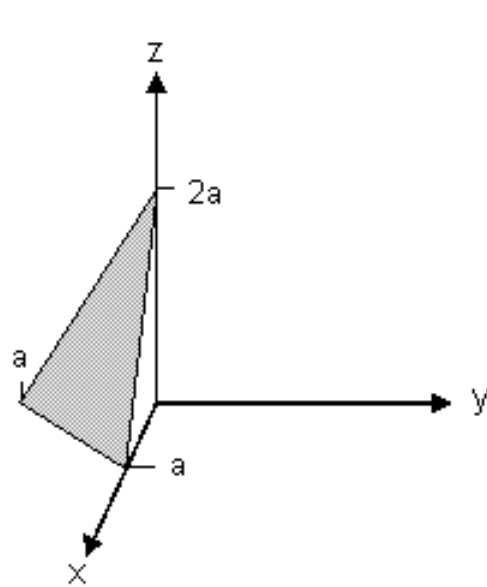
- Establish the coordinate axes along the edges of the unit cell.
- Note where the plane intercepts the axes.
- Divide each intercept by the unit cell length along the respective coordinate axis.
- Record the normalized intercepts in x,y,z order.
- Compute the reciprocal of each intercept.
- Multiply the intercepts by the smallest overall constant that yields whole numbers.

Miller Indices: Example



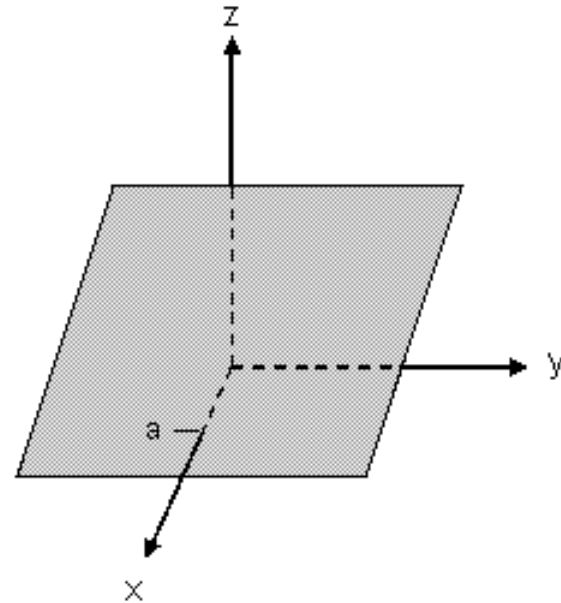
- Normalized intercepts:
 - 1, 2, 3
- Reciprocals:
 - 1, 1/2, 1/3
- Multiplier is 6
- Miller indices for this plane:
 - (6, 3, 2)

Miller Indices: Special Cases



Place a bar over negative intercept.

Miller indices: $(2, \bar{2}, 1)$



When a plane does not intersect an axis the intercept is infinity and the miller index is zero.

Miller indices: $(1, 0, 1)$

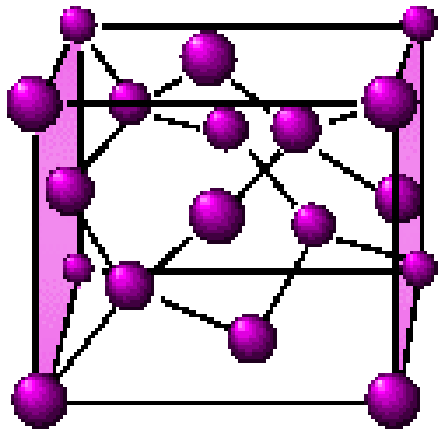
Miller Indices of a Vector

- Establish the coordinate axes along the edges of the unit cell.
- Draw a vector in the direction of interest.
- Decompose the vector into components by projecting it onto the coordinate axes.
- Record the components in x,y,z order.
- Multiply the components by the smallest overall constant that yields whole numbers.
- Miller indices of a vector are enclosed in brackets.
- A plane has the same miller indices as its normal vector.

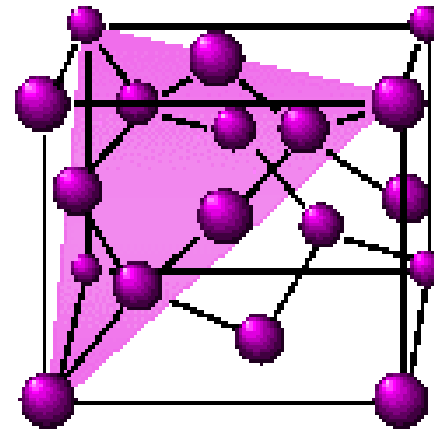
Miller Indices: Recap

- (100) for planes
- $\{100\}$ for all equivalent planes, where in diamond lattice the following six planes are equivalent owing to lattice symmetry (100) , (010) , (001) , $(\bar{1}00)$, $(0\bar{1}0)$ and $(00\bar{1})$
- $[100]$ for vectors
- $\langle 100 \rangle$ for equivalent vectors
- in cubic materials, (hkl) and $[hkl]$ are perpendicular

Crystal Planes



(1,0,0) planes

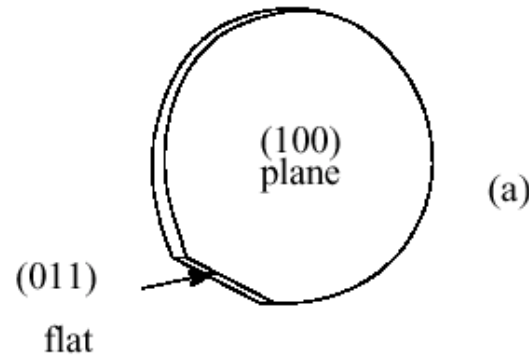


(1,1,1) planes

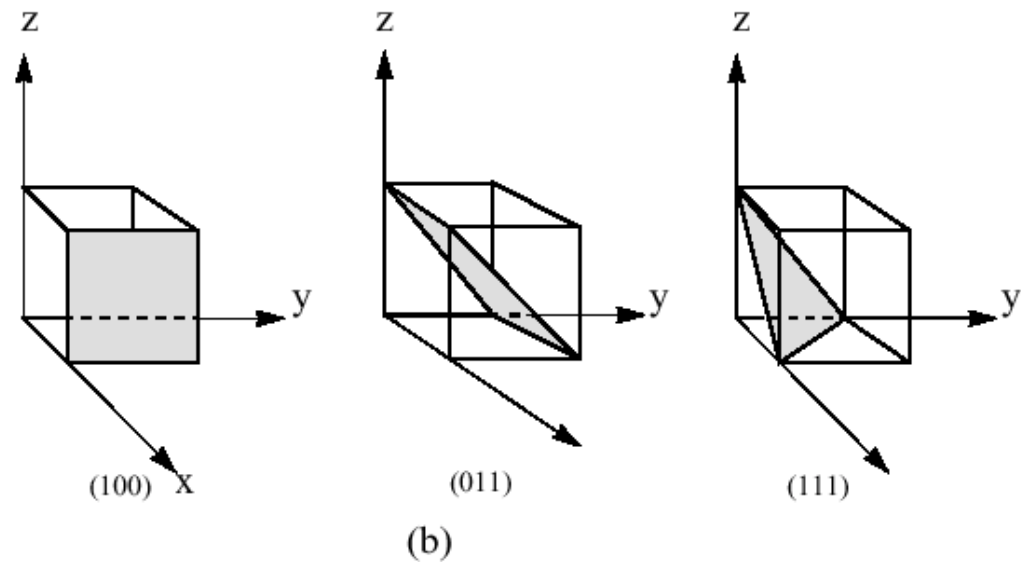
Different chemical and electrical properties.
e.g.: oxidation rate, interface density. →
capacitances and currents.

Silicon Wafer and Crystal Planes

(a) Silicon wafer cut at the (100) plane with a (011) flat to help orient the wafer during IC fabrication.



(b) The standard notation for crystal planes is illustrated.



Crystal Growth

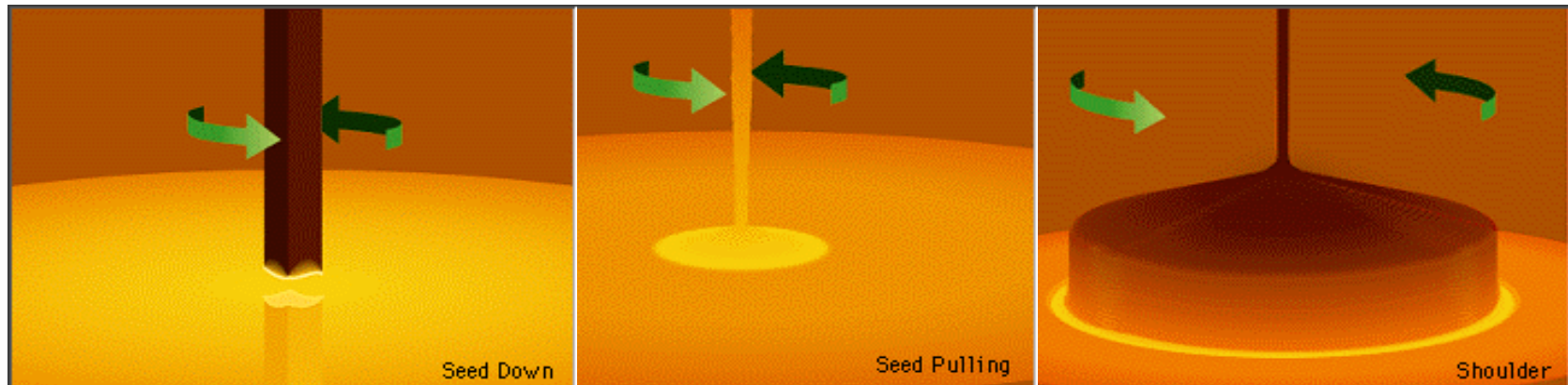
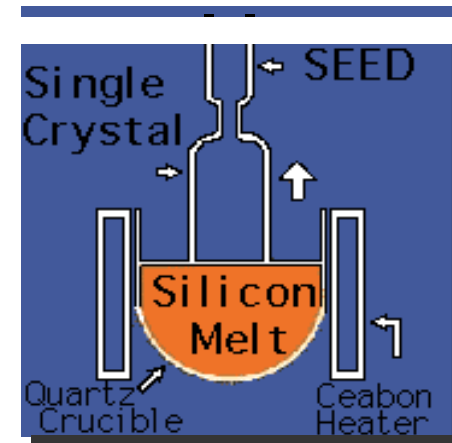
- Silicon never occurs alone in nature → it is a man-made material. Heating SiCl₄ in a hydrogen atmosphere to yield pure Si (polycrystalline)



- Two methods to turn polycrystalline silicon into single crystalline silicon ingot.
 - Czochralski (CZ).
 - Float zone (FZ).

Czochralski (CZ)

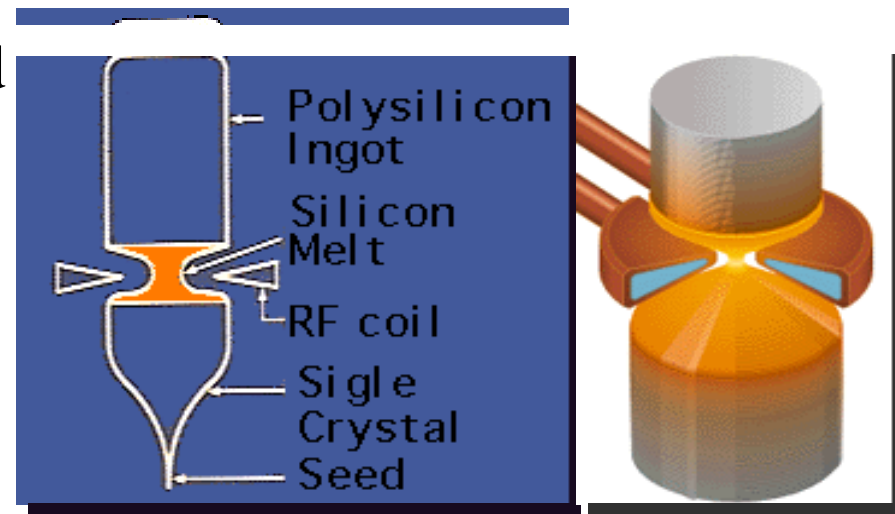
- Melt high purity silicon in a quartz crucible.
- Dips one end of seed on the molten liquid.
- Seed is slowly rotated and pulled.
- By controlling temperature difference, the seed crystal slowly grows.



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Float-zone (FZ)

- Keep poly-Si rod and seed crystal vertically face to face.
- Partially melt by inducted heating from high RF power.
- Molten zone is rotated and gradually moved up.
- The entire polycrystalline rod is converted to single crystal.



<http://www.msil.ab.psiweb.com/english/msilhist0-e.html>

Commonly Used Silicon Wafer Sizes

- 5 inches (125mm):
 - Used in low-end products and research.
- 8 inches (200mm):
 - Commonly used silicon wafer size in production.
- 12 inches (300mm):
 - Prototype IC fabricated with this wafer size demonstrated this year. It will gradually be used in full production.

To Probe Further

- Reading assignment:
 - Pierrer & Neudeck Volume-1 chapter-1
- References:
 - Streetman chapter-1
 - Silicon process VLSI
 - Semiconductor applet services @ SUNY buffalo
 - <http://jas2.Eng.Buffalo.edu/applets/>
 - **Mitsubishi materials silicon:**
 - <http://www.msil.ab.psiweb.com/english/index-e.html>