COLUMBIA | ENGINEERING
The Fu Foundation School of Engineering and Applied Science

ELEN 3106/4106 Lecture 2

Semiconductors and Crystal Properties

Outline

- Define semiconductors
- Crystal properties
- Crystal lattices
- Structure and orientation in Si
- Miller indices

Assignments:

Reading: Streetman and Banerjee §1.1, 1.2. Review Ch. 2 as necessary

Homework 1 due Friday Sept 12th by 5pm

Common semiconductor materials

- Semiconductors can be single element, like ___ or ___
- Or compound element, like _____
- Or an alloy, such as $Al_xGa_{(1-x)}N$ where x is the _____of the particular element

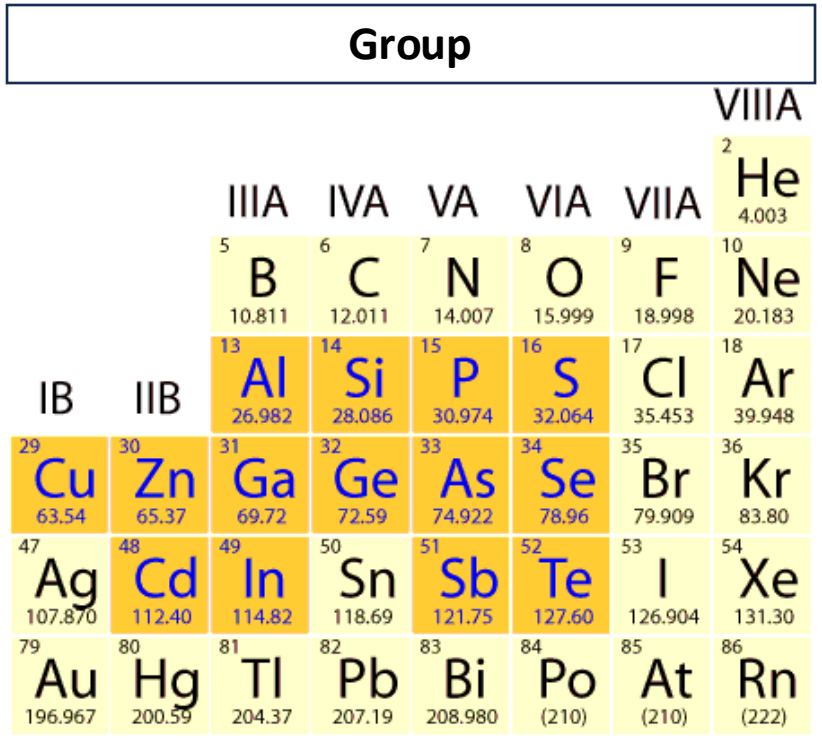


Image Credits: PV Education

Common semiconductor materials

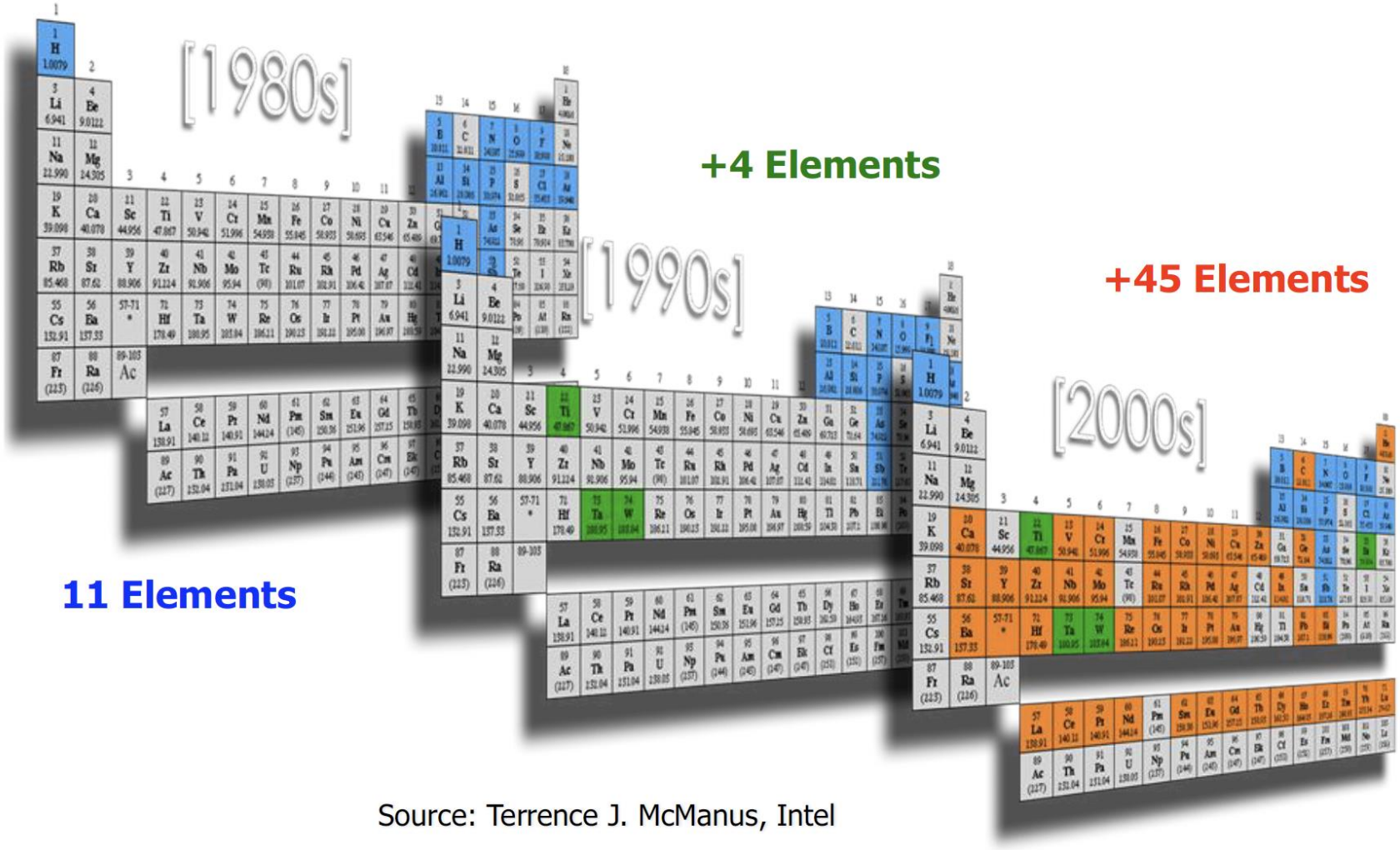
- Common semiconductors and their properties

		E_g (eV)	μ_n (cm^2/V-s)	μ_p (cm^2/V-s)	m_n^*/m_o (m_l,m_t)	m_p^*/m_o (m_{lh},m_{hh})	a (Å)	ϵ_r	Density (g/cm^3)	Melting point (°C)
Si	(*i*/*D*)	1.11	1350	480	0.98, 0.19	0.16, 0.49	5.43	11.8	2.33	1415
Ge	(*i*/*D*)	0.67	3900	1900	1.64, 0.082	0.04, 0.28	5.65	16	5.32	936
SiC (α)	(*i*/*W*)	2.86	500	—	0.6	1.0	3.08	10.2	3.21	2830
AlP	(*i*/*Z*)	2.45	80	—	—	0.2, 0.63	5.46	9.8	2.40	2000
AlAs	(*i*/*Z*)	2.16	1200	420	2.0	0.15, 0.76	5.66	10.9	3.60	1740
AlSb	(*i*/*Z*)	1.6	200	300	0.12	0.98	6.14	11.0	4.26	1080
GaP	(*i*/*Z*)	2.26	300	150	1.12, 0.22	0.14, 0.79	5.45	11.1	4.13	1467
GaAs	(*d*/*Z*)	1.43	8500	400	0.067	0.074, 0.50	5.65	13.2	5.31	1238
GaN	(*d*/*Z*, *W*)	3.4	380	—	0.19	0.60	4.5	12.2	6.1	2530
GaSb	(*d*/*Z*)	0.7	5000	1000	0.042	0.06, 0.23	6.09	15.7	5.61	712
InP	(*d*/*Z*)	1.35	4000	100	0.077	0.089, 0.85	5.87	12.4	4.79	1070
InAs	(*d*/*Z*)	0.36	22600	200	0.023	0.025, 0.41	6.06	14.6	5.67	943
InSb	(*d*/*Z*)	0.18	10^5	1700	0.014	0.015, 0.40	6.48	17.7	5.78	525
ZnS	(*d*/*Z*, *W*)	3.6	180	10	0.28	—	5.409	8.9	4.09	1650*
ZnSe	(*d*/*Z*)	2.7	600	28	0.14	0.60	5.671	9.2	5.65	1100*
ZnTe	(*d*/*Z*)	2.25	530	100	0.18	0.65	6.101	10.4	5.51	1238*
CdS	(*d*/*W*, *Z*)	2.42	250	15	0.21	0.80	4.137	8.9	4.82	1475
CdSe	(*d*/*W*)	1.73	800	—	0.13	0.45	4.30	10.2	5.81	1258
CdTe	(*d*/*Z*)	1.58	1050	100	0.10	0.37	6.482	10.2	6.20	1098
PbS	(*i*/*H*)	0.37	575	200	0.22	0.29	5.936	17.0	7.6	1119
PbSe	(*i*/*H*)	0.27	1500	1500	—	—	6.147	23.6	8.73	1081
PbTe	(*i*/*H*)	0.29	6000	4000	0.17	0.20	6.452	30	8.16	925

All values at 300 K. *Vaporizes

Image Credits: Textbook (Appendix III)

Material complexity has been increasing

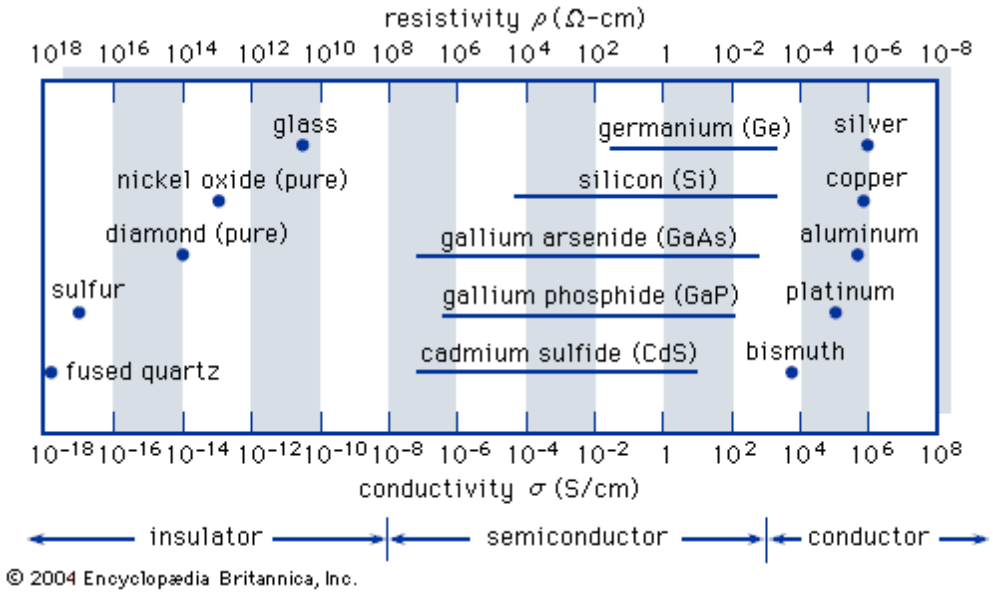


Source: Terrence J. McManus, Intel

Image Credits: Terence J. McManus, Intel

What makes a semiconductor?

- _____ are between metals and insulators
- Produce only small amount of _____ that are free to move
- Semiconductors are *usually* _____ solids
  - Why? Single-crystals give long-range order
- Atomic arrangements in solids:
  - Crystalline: atoms arranged in a _____
  - Polycrystalline: many small regions of single-crystal
  - Amorphous: no periodic structure at all



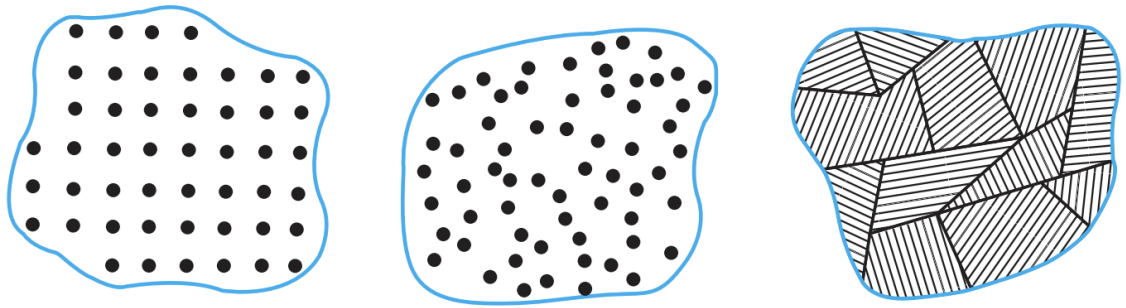
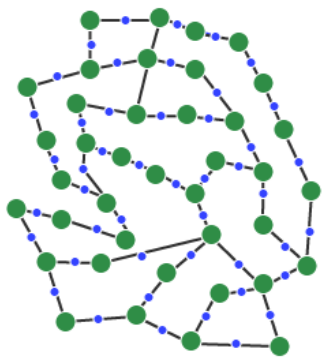


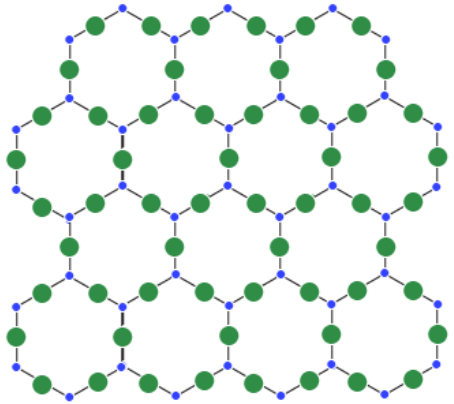
Image Credits: Britannica, Textbook

Crystalline Solids

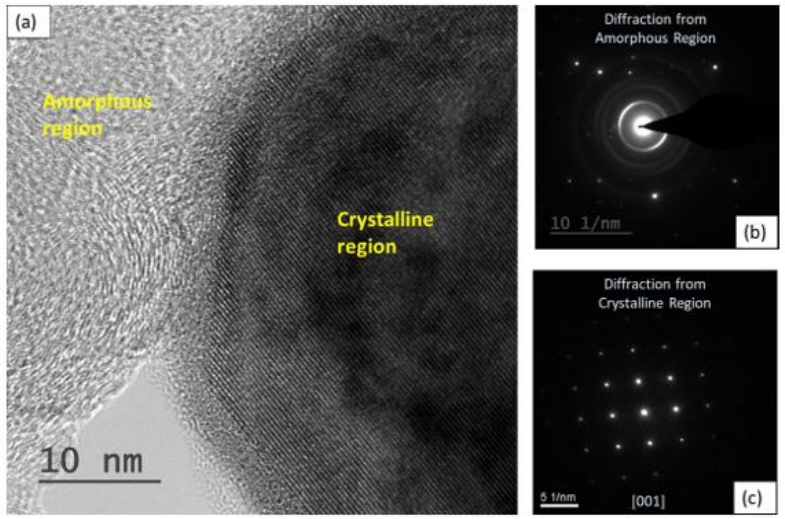
- Crystals have long range order and symmetry, known as _____
- The basic arrangement of atoms repeated throughout the crystal is called the _____
- Specific arrangement of atoms in each semiconductor are of critical importance!



Amorphous Solids



Crystalline Solids

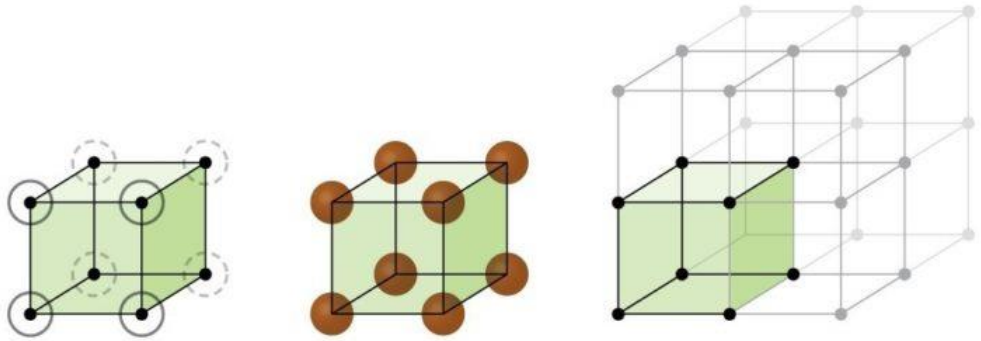


TEM image showing interface between amorphous and crystalline regions. Crystalline region shows distinct parallel lines (or row of atoms), whereas the amorphous region does not.

Image Credits: GeeksForGeeks, Virtual Labs

Crystal Lattice

- A _____ of particles (either atoms, molecules, or ions) in a crystalline solid
- The lattice is a repetitive pattern that extends throughout the entire crystal
- This repeating pattern is called the _____



Source: Lumen learning

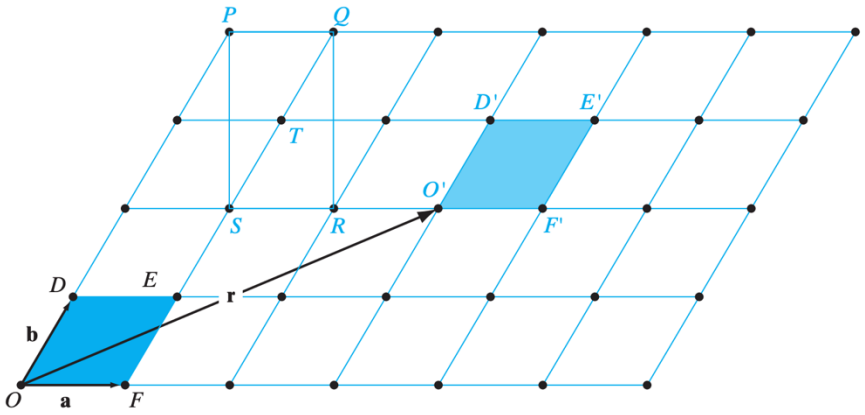
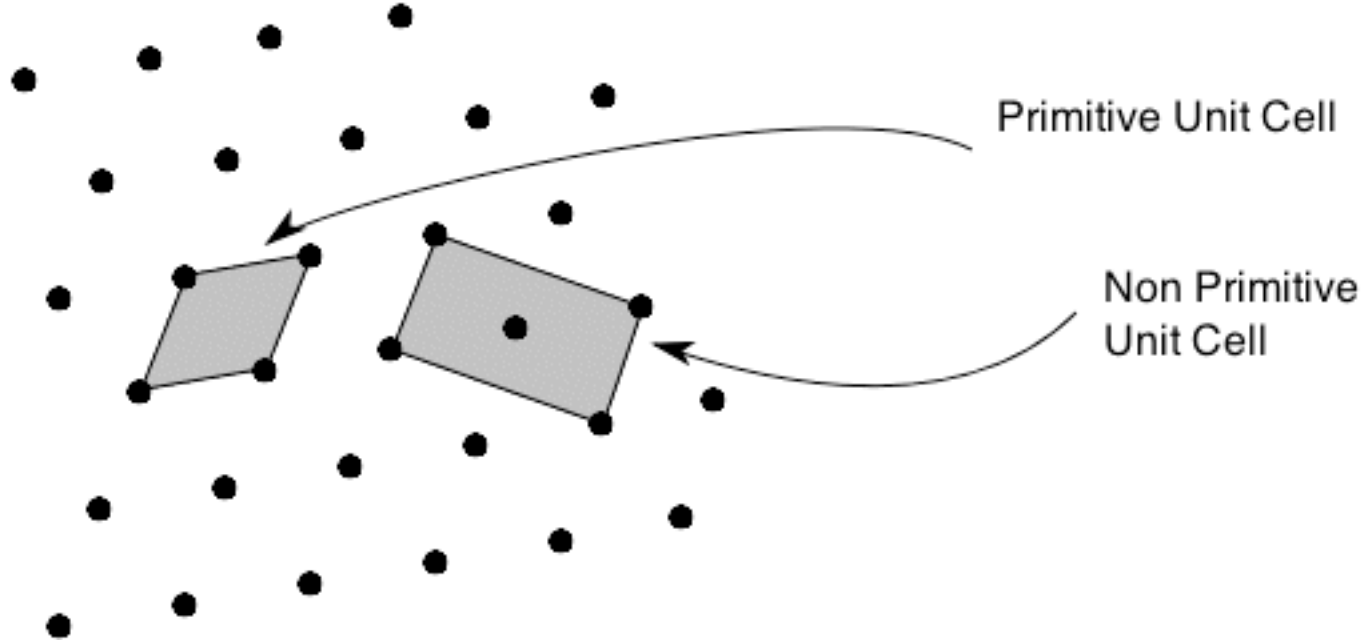


Figure 1–2
A two-dimensional lattice showing translation of a unit cell by r = 3a + 2b.

Source: Textbook

Primitive Unit Cell

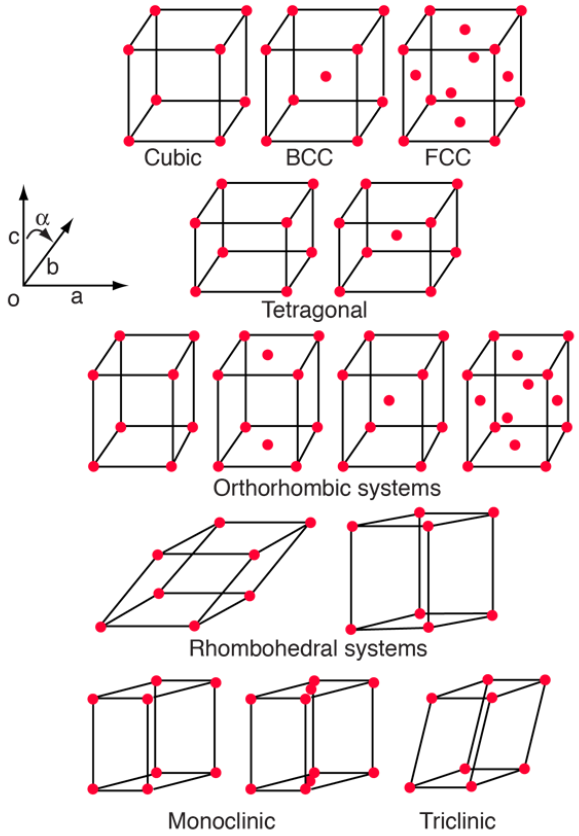
- The fundamental building block of a lattice is a primitive cell with _____ at its _____
- Sometimes it is easier to describe the crystal in terms of a larger “unit” cell with lattice points not only at the corners but also at body or face centers
- Is there only every one particle on a lattice point?



Source: University of Cambridge

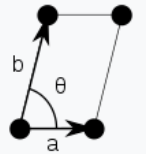
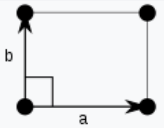
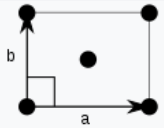
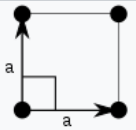
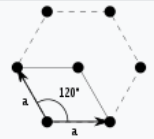
Bravais Lattices

In 3-D, these are _____ Bravais lattices.



Source: Hyperphysics

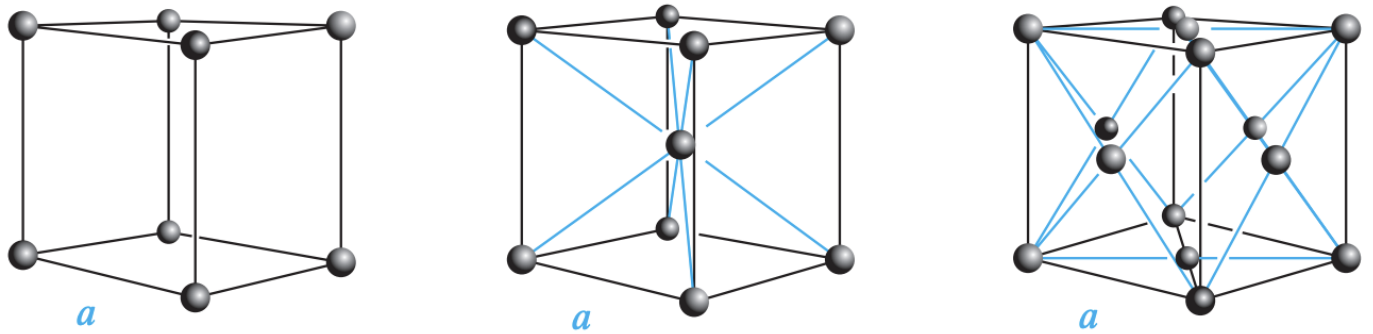
In 2-D, there are ____.

Lattice system	Point group (Schönflies notation)	5 Bravais lattices	
		Primitive (p)	Centered (c)
Monoclinic (m)	C_2	 Oblique (mp)	
Orthorhombic (o)	D_2	 Rectangular (op)	 Centered rectangular (oc)
Tetragonal (t)	D_4	 Square (tp)	
Hexagonal (h)	D_6	 Hexagonal (hp)	

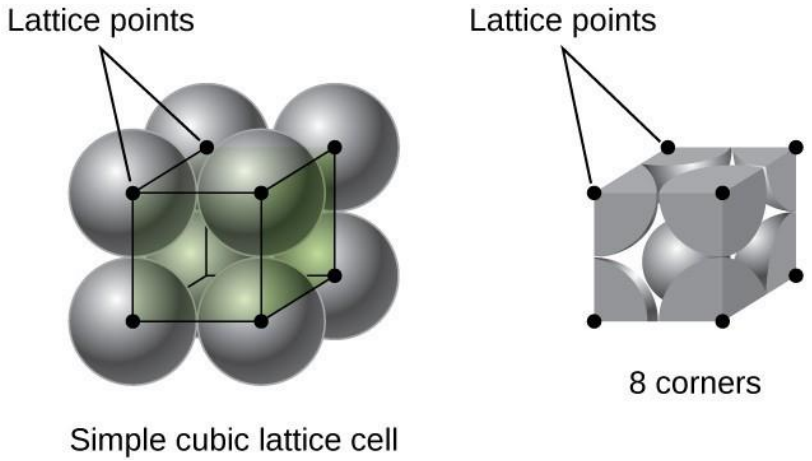
Source: Wikipedia

Cubic Lattices

- Let's look at the case where the crystal lattice unit cell is a _____
- *a* is called the _____: the length of one side of the cube
  - Units: Angstrom (Å)
- The arrangement of particles at each lattice point is called the _____
- 3 types of cubic lattice structures:



Source: Textbook



Source: Lumen learning

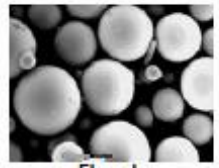
The Scale of Things – Nanometers and More

Things Natural

Dust mite
200 µm

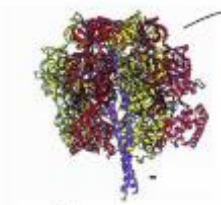
Ant
~ 5 mm

Human hair
~ 60-120 µm wide

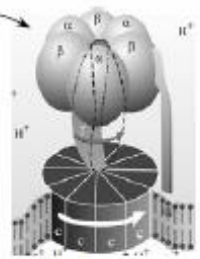


Fly ash
~ 10-20 µm

Red blood cells
(~7-8 µm)



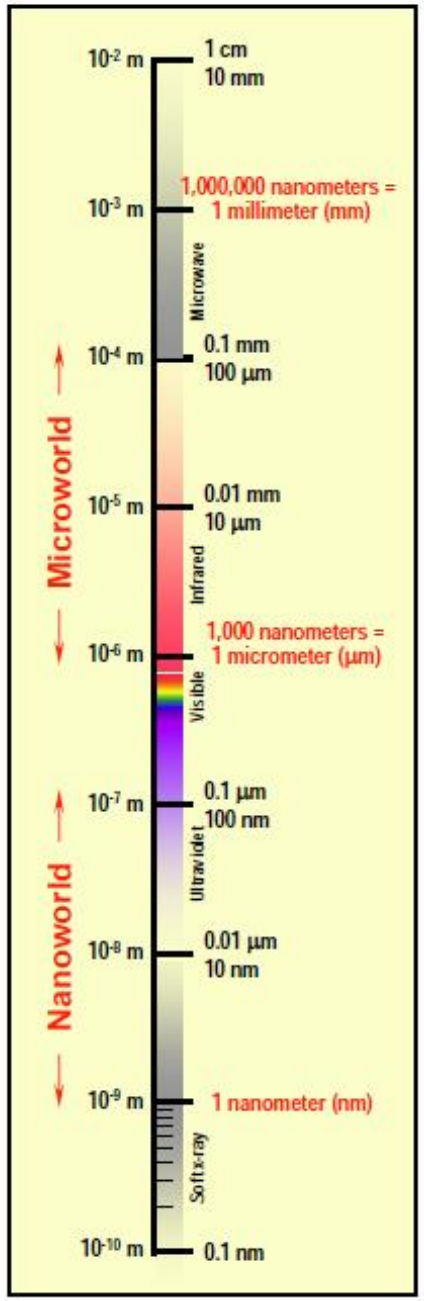
~10 nm diameter



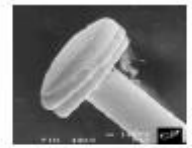
ATP synthase

DNA
~2-1/2 nm diameter

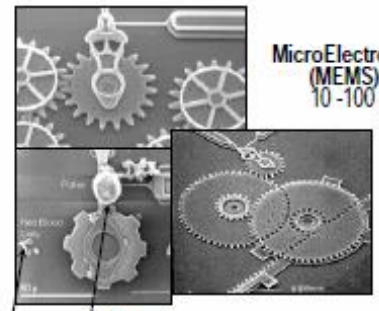
Atoms of silicon
spacing 0.078 nm



Things Manmade

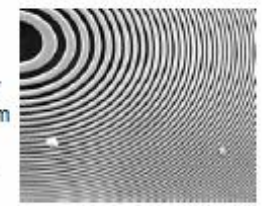


Head of a pin
1-2 mm

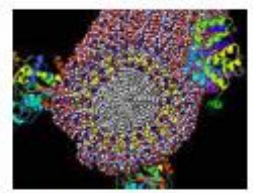


MicroElectroMechanical
(MEMS) devices
10 -100 µm wide

Pollen grain
Red blood cells

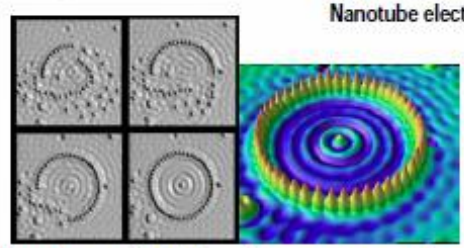


Zone plate x-ray "lens"
Outer ring spacing ~35 nm

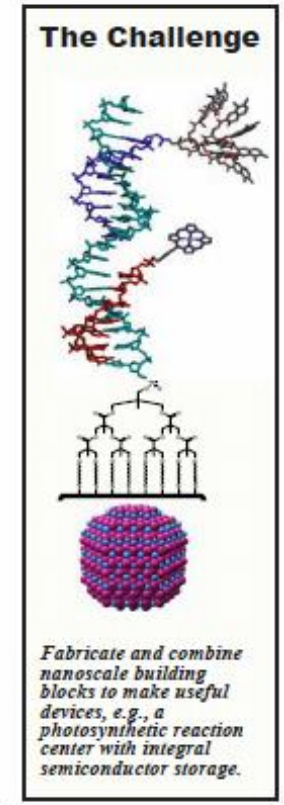


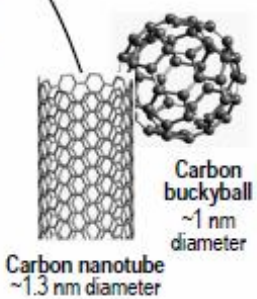
Self-assembled,
Nature-inspired structure
Many 10s of nm

Nanotube electrode



Quantum corral of 48 iron atoms on copper surface
positioned one at a time with an STM tip
Corral diameter 14 nm



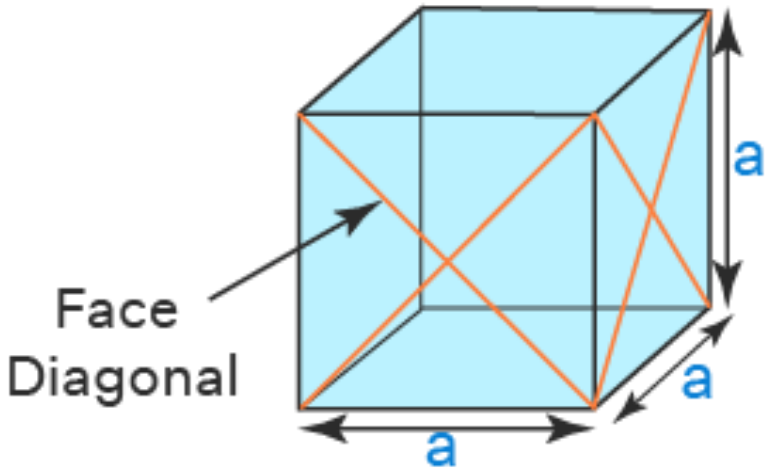


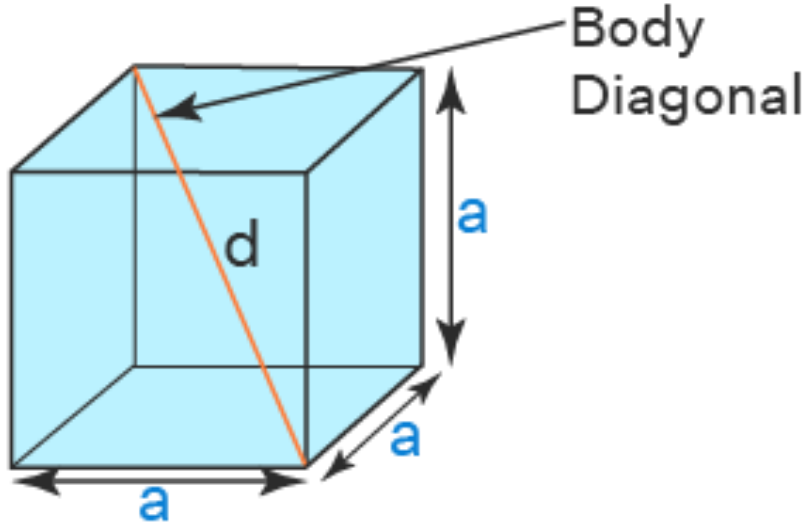
Carbon
buckyball
~1 nm
diameter

Carbon nanotube
~1.3 nm diameter

Recall: Cube Lengths, Diameters, and Volumes

- Length of an edge = _____
- Length of a face diagonal = _____
- Length of a body diagonal = _____



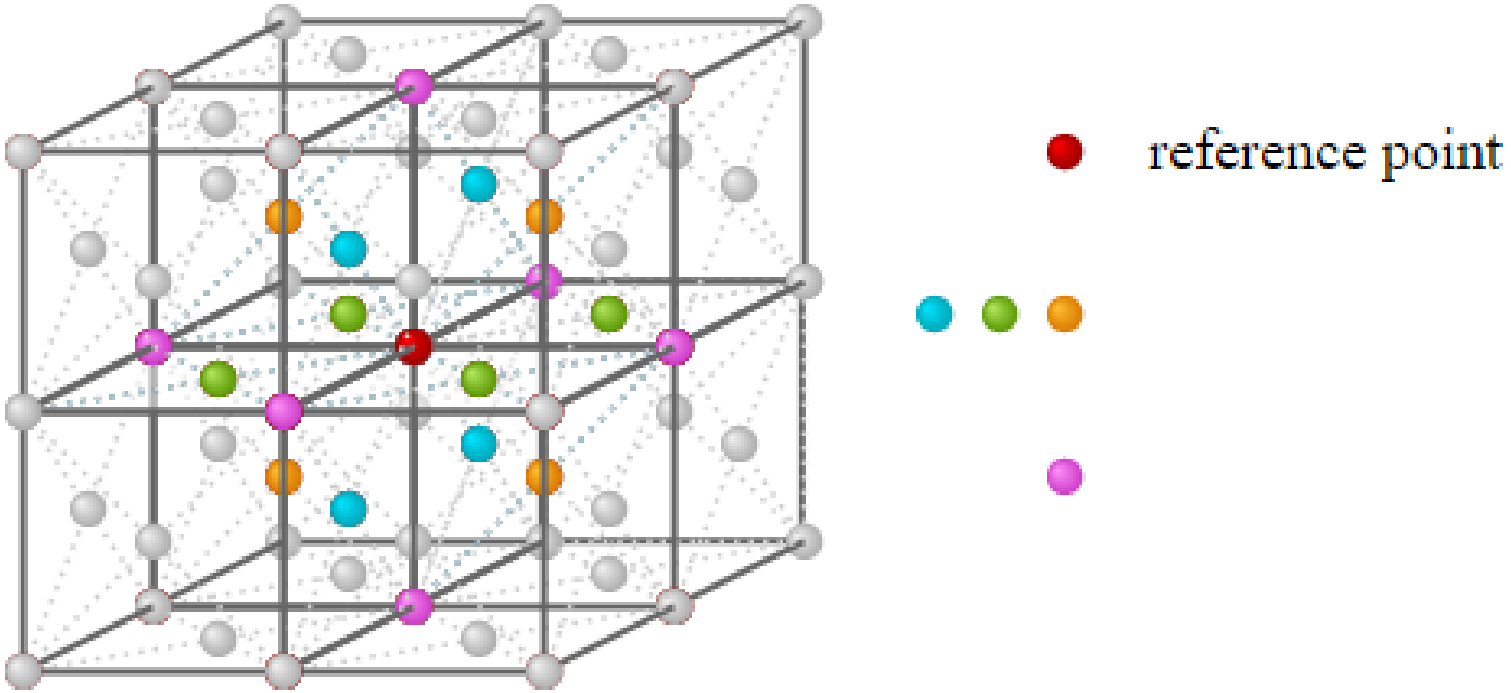


- Volume of cube = _____

Source: Cuemath

Nearest Neighbor

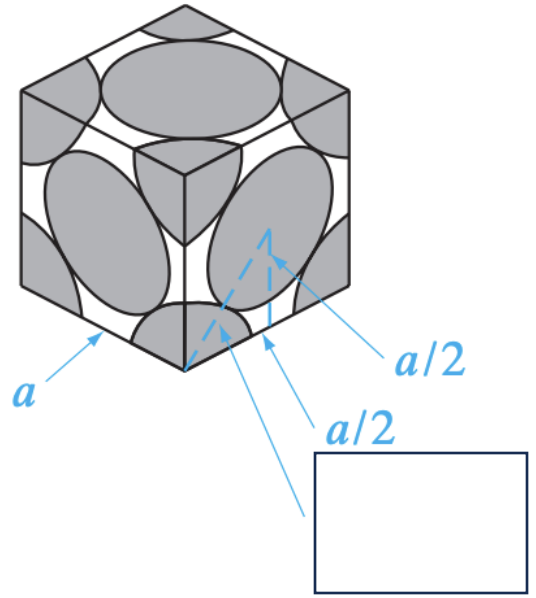
- What is the unit cell? _____
- Taking a corner atom as the reference
  - How many nearest neighbors? _____
  - How many next-nearest neighbors? _____



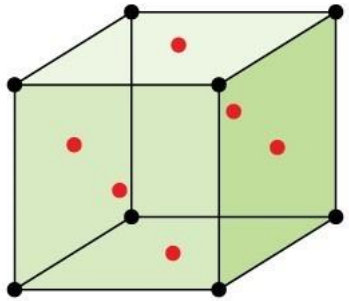
Source: Physics LibreText

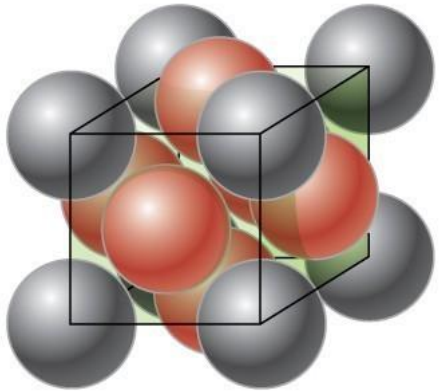
Hard Sphere Approximation

- How do we “stuff” particles into unit cells?
  - We can approximate the atoms as hard spheres, packed into the unit cell
- Assume atoms are _____
- Question: Can we find the fraction of the fcc unit cell volume filled with hard spheres (_____), assuming a = 5 Å?
  - Nearest neighbor distance?

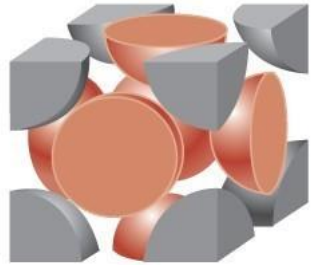


Source: Textbook





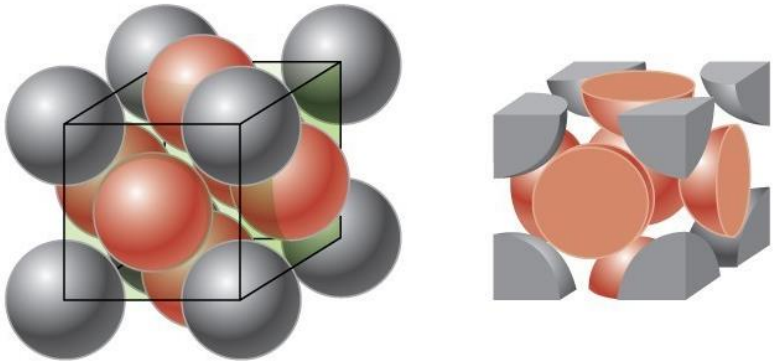
Face-centered cubic structure



Source: Lumen learning

Atomic Packing Factor

- Radius of atom?



Face-centered cubic structure

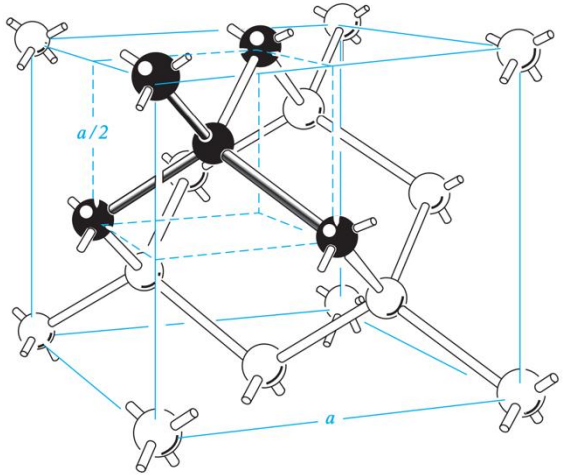
- # of atoms per unit cell?

- Packing Factor? Ratio of the volume occupied by the average number of atoms in a unit cell to the total volume of the unit cell
  - (# of _____ × Volume of an _____/ Volume of _____)

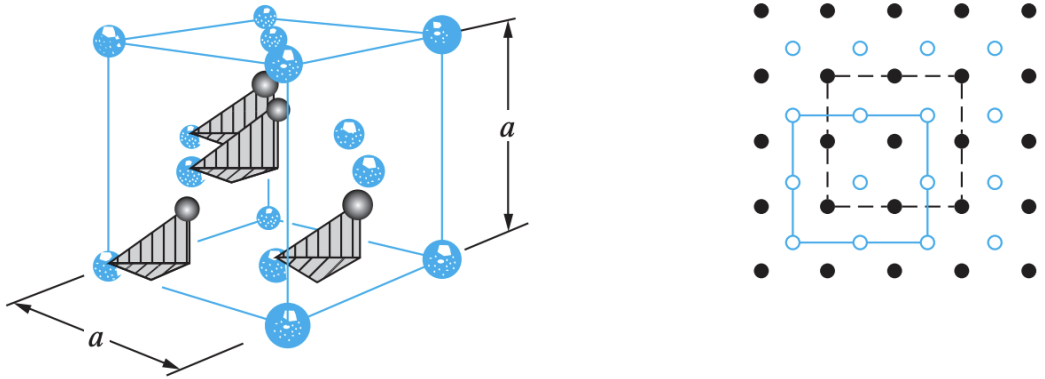
Source: Lumen learning

Si Crystal Lattice

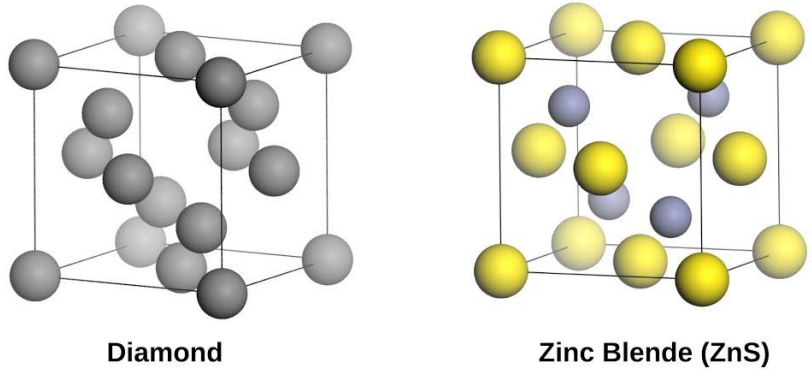
- _____ lattice
  - a = _____ Å
  - fcc lattice with basis of _____
  - AKA, fcc lattice with an extra atom placed at **a**/4 + **b**/4 + **c**/4 from each of the fcc atoms!
- Many compound semis are in diamond structure w/ interpenetrating fcc
  - Called _____ lattice



Diamond crystal lattice showing 4 nearest neighbors. Source: Textbook



Diamond crystal lattice, atoms placed at ¼, ¼, ¼ from each fcc atom. Top view on the right. Source: Textbook



Diamond and Zinc Blende crystal lattices. Source: Delta Studio

Helpful link on visualizing lattices

https://www.ibiblio.org/e-notes/Cryst/Cryst.htm

Basis versus lattice point clarification

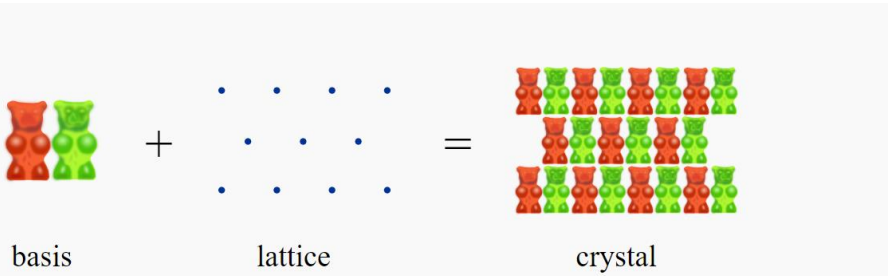
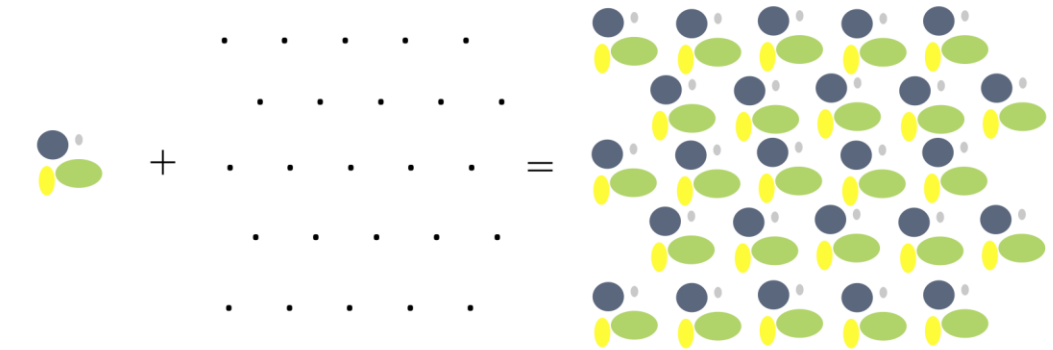


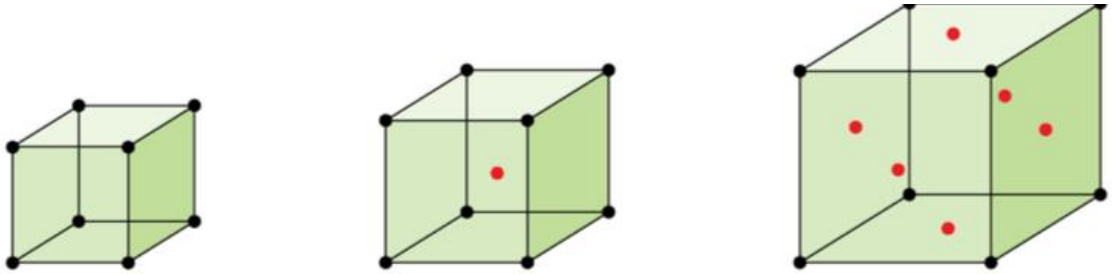
Fig. 3 - A crystal is defined as a lattice with a basis added to each lattice site. Usually the basis consists of an atom, a group of atoms or a molecule.

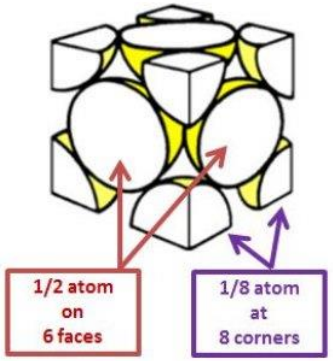


Source: Physics-in-a-nutshell, WordPress

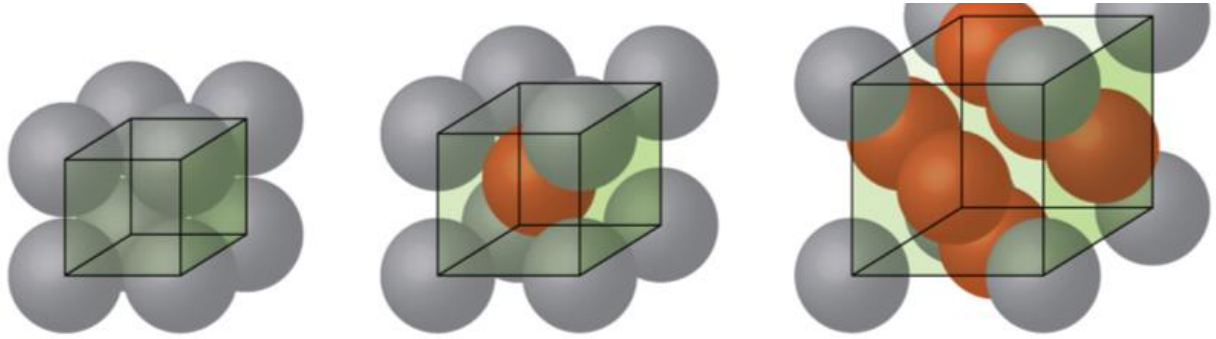
Further Info on Cubic Lattices

Total # of lattice points in unit cell?





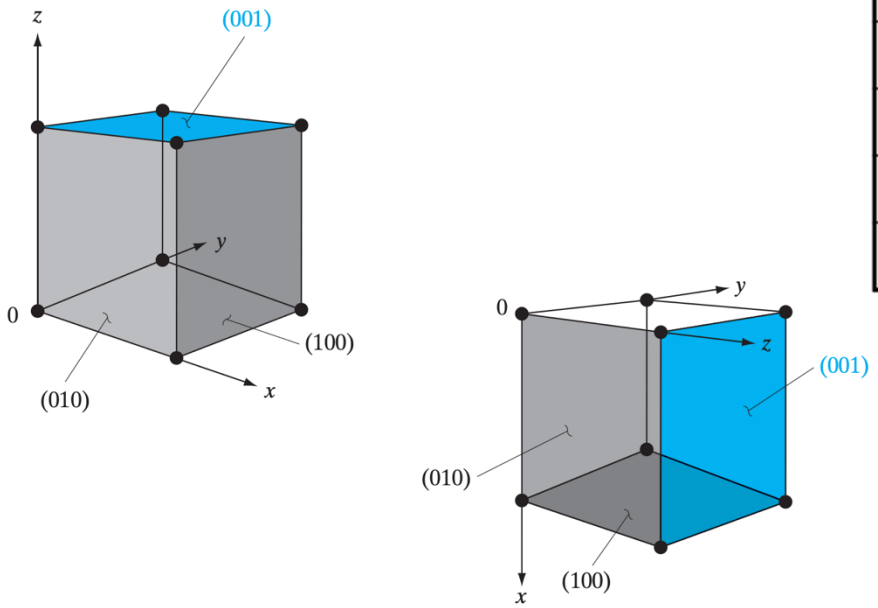
Total # of atoms in unit cell?



Source: University of Wisconsin

Crystal Planes and Directions

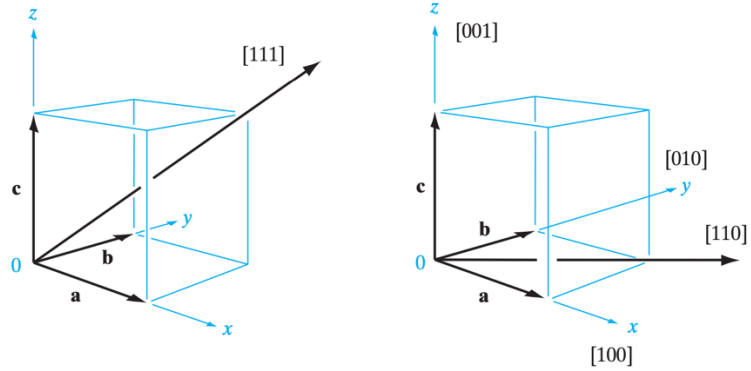
- Described using _____ coordinate system
- _____ are the three integers (*hkl)* that define a set of parallel plans



Notation	Interpretation
(*h k l*)	crystal plane
{ *h k l* }	equivalent planes
[*h k l*]	crystal direction
< *h k l* >	equivalent directions

***h*: inverse *x*-intercept of plane**
***k*: inverse *y*-intercept of plane**
***l*: inverse *z*-intercept of plane**

{100} planes equivalent by rotation. Source: Textbook



Crystal directions. Notation similar to vector components. Source: Textbook

How to Find Miller Indices

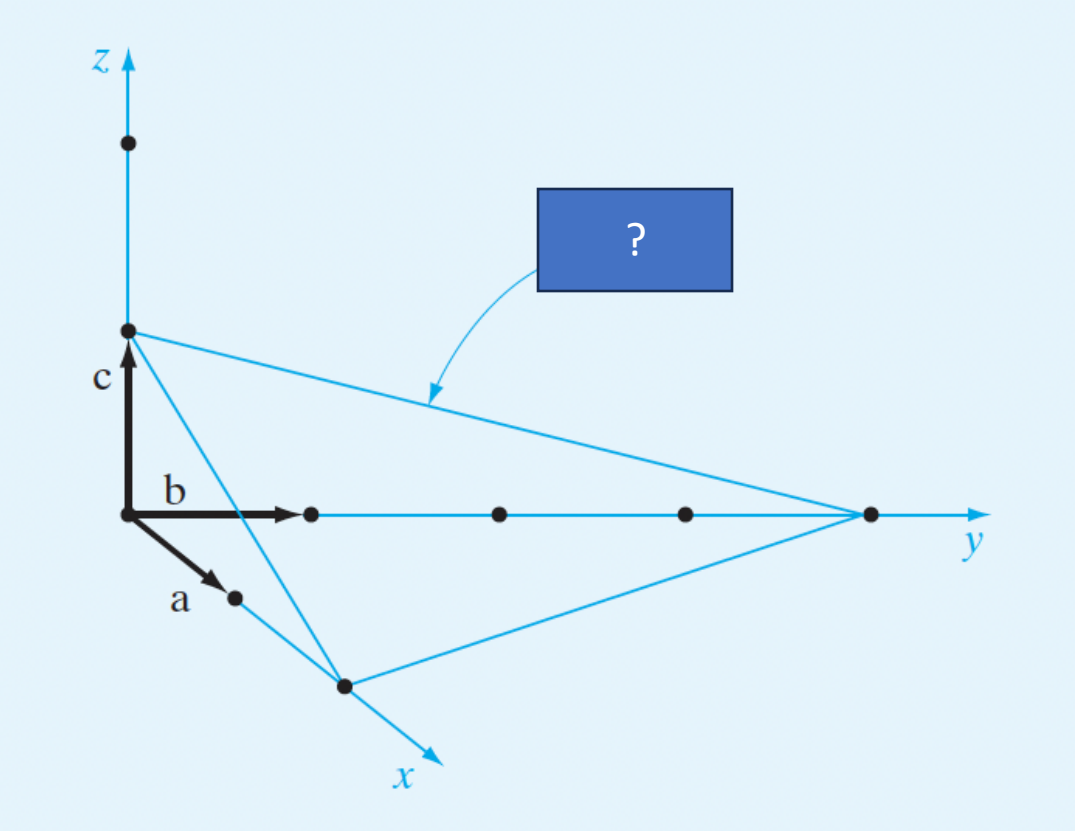
The three integers describing a particular plane are found in the following way:

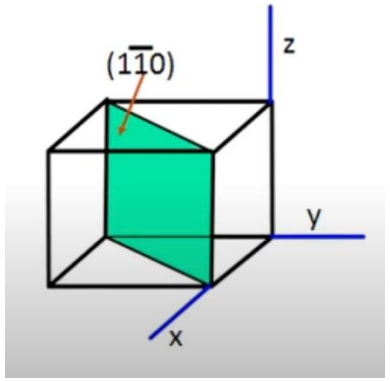
1. Find the intercepts of the plane with the crystal axes

1. Take the reciprocals of the three integers found in step 1 and reduce these to the smallest set of integers h, k, and l

1. Label the plane (hkl).

- Note: if the intercept is negative, we put a ___ over it
- A _____ in a Miller index indicates that the plane is parallel to the axis (intercept is _____)

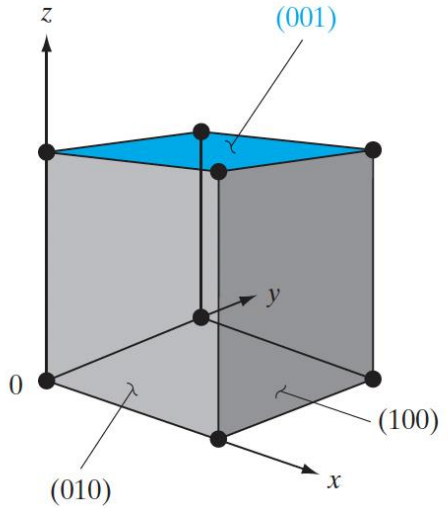




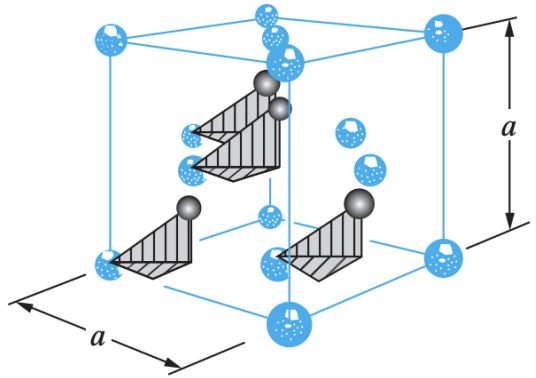
Source: Textbook, Youtube

Volume and Areal Densities

- Calculate the areal density of Si atoms (number of atoms/cm^2) on the (100) plane, given that the lattice constant of Si is 5.43 Å.

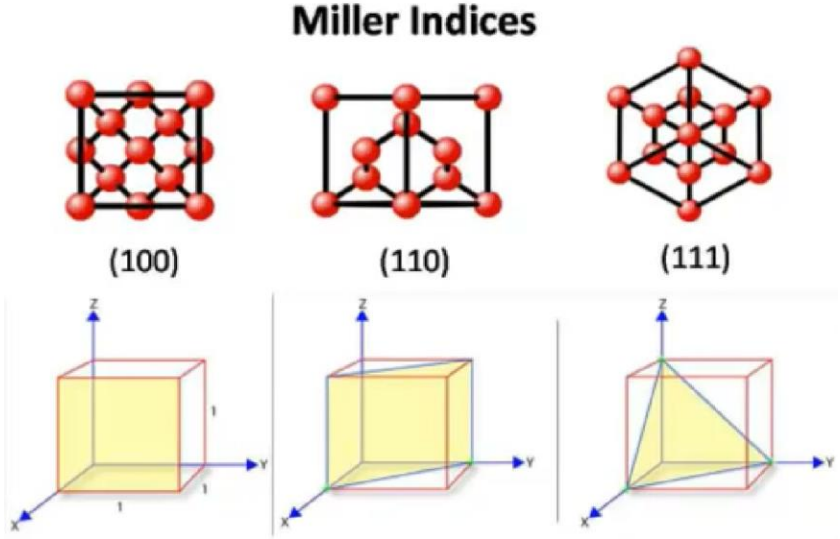


- Calculate the volume density of Si atoms (number of atoms/cm^3).

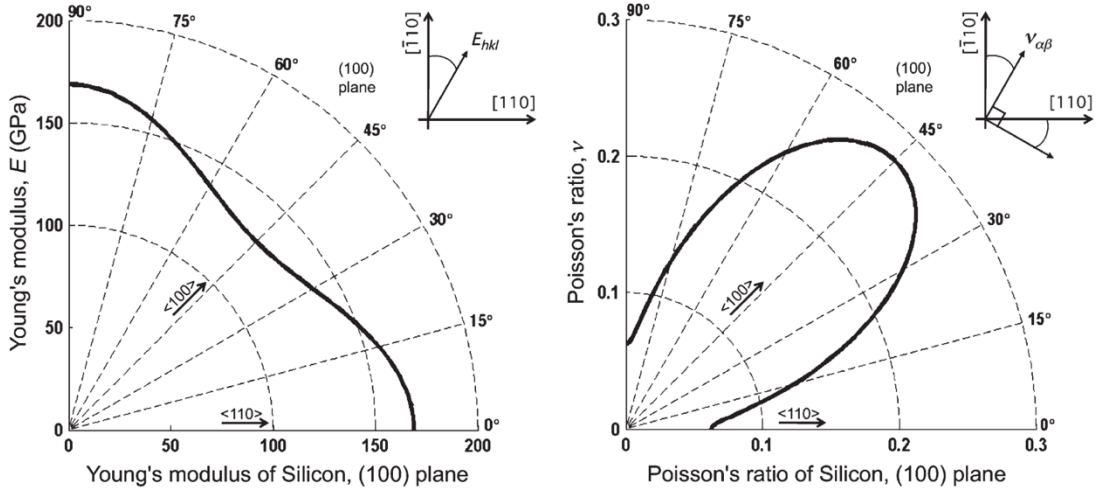


Wafer Orientation

- Semiconductor _____ surfaces are preoriented along a chosen crystallographic plane
- Certain _____ steps and performance in some types of devices depend on orientation
- Orientation effects can greatly influence the conductivity, _____, optical, and thermal properties



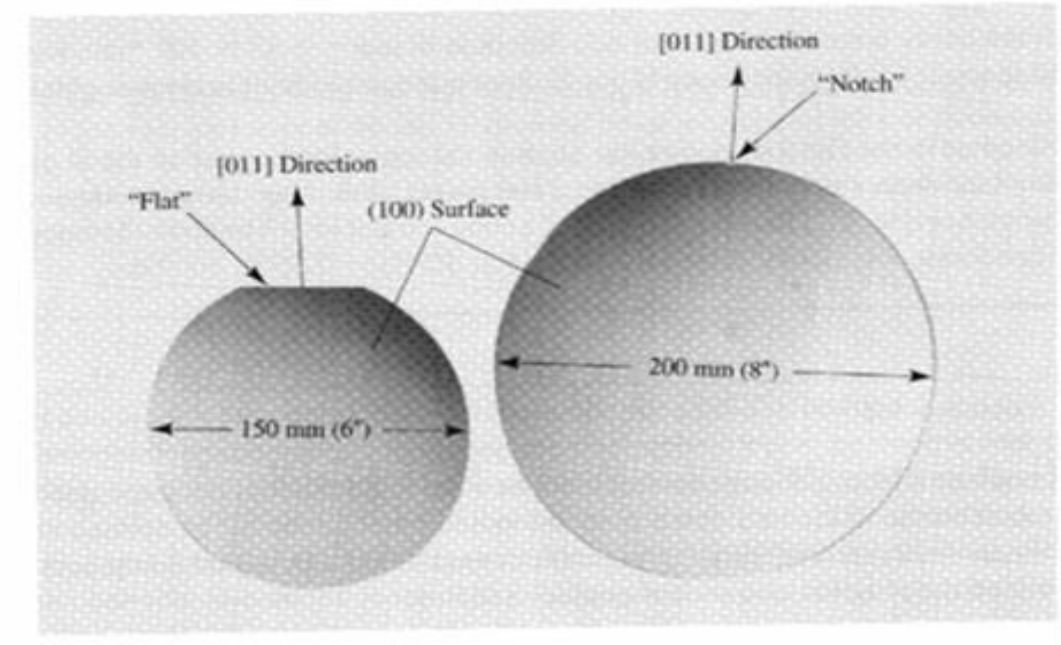
Miller indices in Si wafers. Source: University Wafer



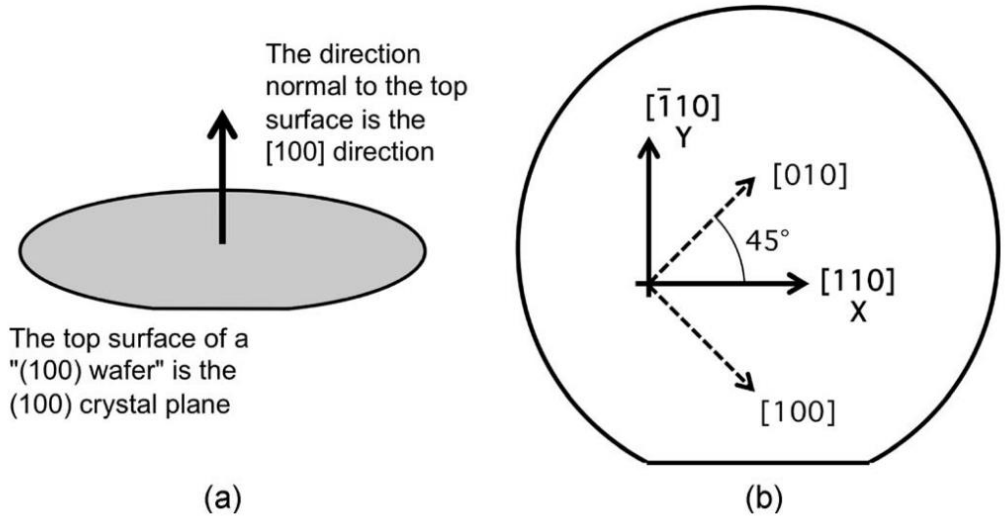
Si mechanical properties, Young's Modulus and Poisson's ratio, versus orientation in the (100) plane. Source: T. Kenny et al., *J. Micromech Microeng* (2010)

Orientation in Si Wafers

- Si wafers typically cut along _____ plane, with _____ or flat denoting reference direction



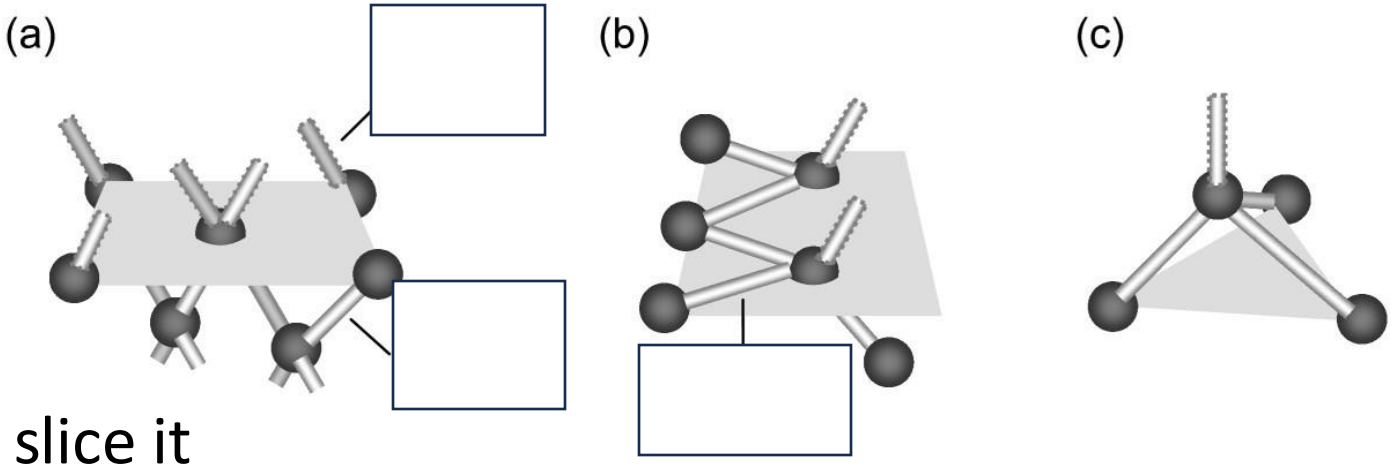
{100} Si wafer. Source: Pierret, *Semiconductor Device Fundamentals*



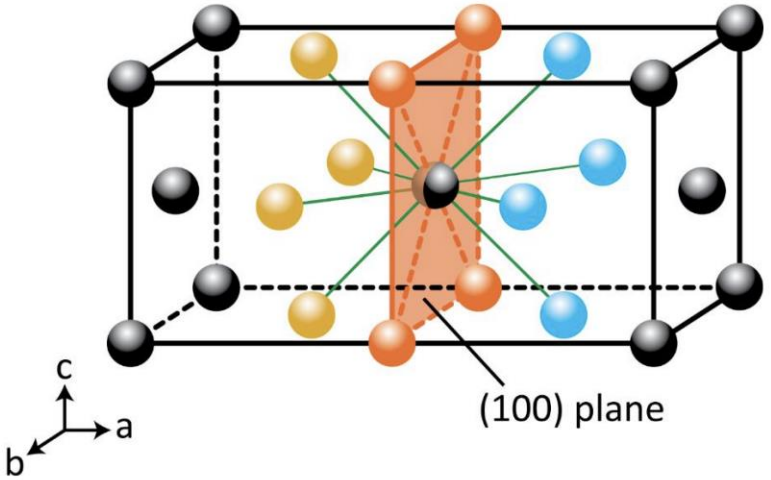
Crystal orientation in 100-mm-diameter silicon wafers. Source: T. Kenny et al., *J. Micromech Microeng* (2010)

Dangling Bonds

- The _____ bonds yielding undercoordinated atoms



- Let's slice a simple fcc lattice and slice it along the _____ plane. How many bonds are broken?



- Broken chemical bonds effect the _____ properties
- Surface ≠ _____
- Can have significant impact in in _____ where surface area to volume ratios are large

Source: Nano Express