Chemistry 1000 Lecture 10: Metals and crystal structures

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Classification of the elements

Element	Appearance	Resistivity/$\Omega\,\mathrm{m}$	Fluoride(s)
Na	silvery solid	4.2×10^{-8}	ionic NaF
Ca	silvery solid	3.9×10^{-8}	ionic CaF_2
Ni	silvery solid	6.8×10^{-8}	ionic NiF_2
Al	silvery solid	2.7×10^{-8}	molecular Al_2F_6
Hg	silvery liquid	9.8×10^{-7}	ionic Hg_2F_2 and HgF_2
Ge	grey solid	4.6×10^{-2}	molecular GeF_4 and GeF_2
Sb	silvery solid	3.9×10^{-7}	molecular SbF_3 and SbF_5
B	black solid	1.8×10^{4}	molecular BF_3
P	white solid	1.0×10^{9}	molecular PF_3, PF_5 and P_2F_4

Metal: malleable, ductile, good conductor of heat and electricity, shiny, resistivity increases with increasing T

Nonmetal: brittle when solid, poor conductor of heat and electricity (insulator)

Metalloid: intermediate between metal and nonmetal, often semiconducting

Semiconductor: electrical conductivity is between that of a conductor and insulator, resistivity decreases with increasing T

Q& A about bonding in metals

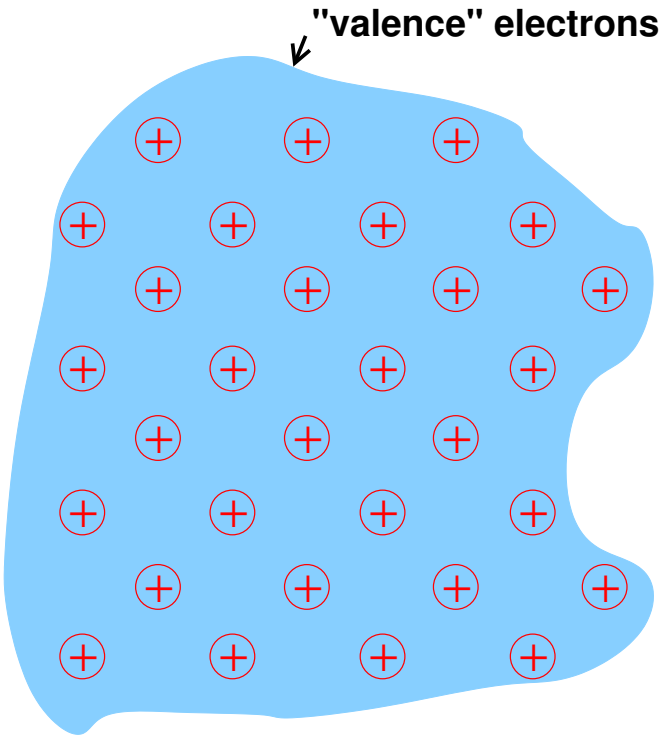
Question: Why do metals conduct electricity?

Answer: They must have free electrons.

Question: On an atomic level, what distinguishes metals from nonmetals?

Answer: Metals give up their electrons relatively easily (low ionization energies).

Quasi-free-electron model of metals



Explains metal

- heat and electrical conductivity
- deformability (ductility, malleability)

Crystal structure of metals

- Metals typically are (poly)crystalline.

Crystal lattice: repeating arrangement of points in space

Polycrystal: a material composed of many microscopic crystals (grains) stuck together in different orientations

Grain boundary: surface where two grains meet

Single crystal: a material composed of a single, (nearly) perfectly ordered crystalline material without grain boundaries

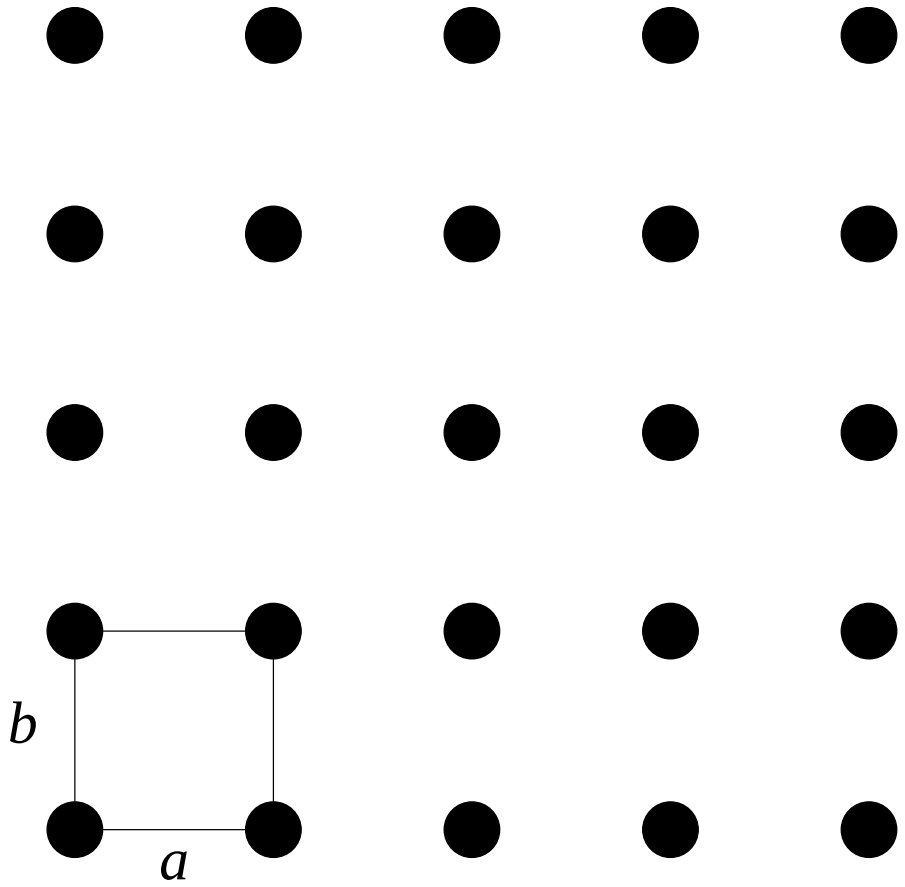
- Even in a polycrystal, relatively few atoms are at the grain boundary so most are surrounded by a well-organized crystal environment.

Unit cells

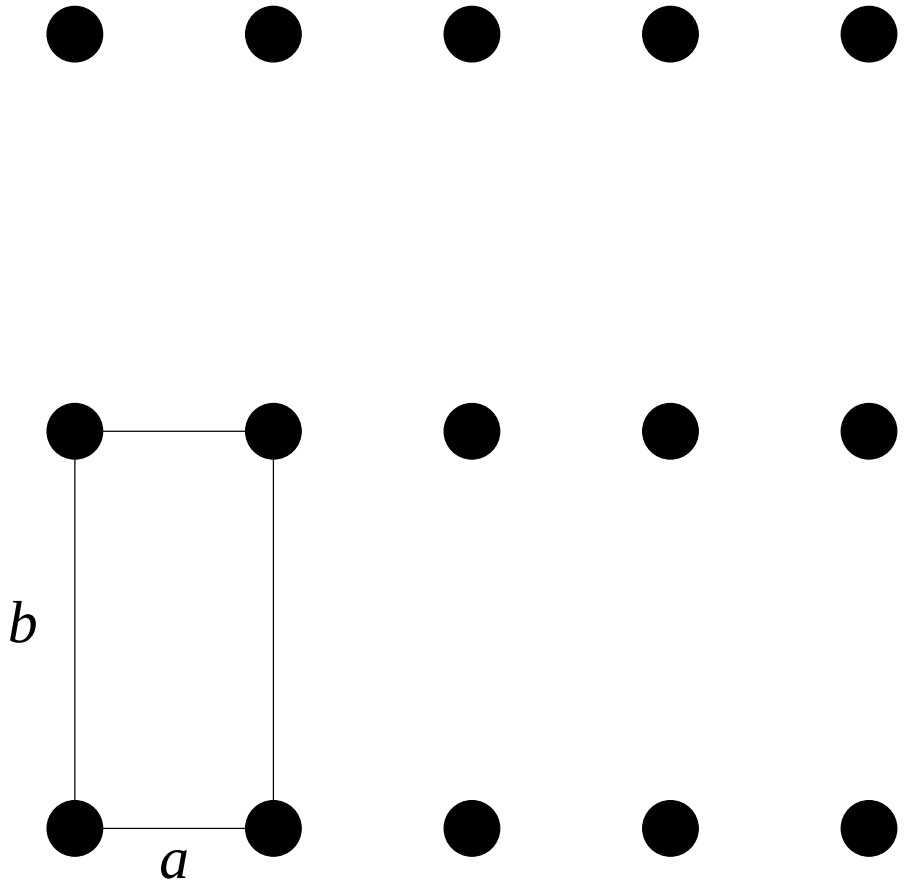
- The lattice can be generated by sliding a unit cell along lattice vectors.
- No rotation or reflection of unit cells is allowed, only sliding.
- The smallest unit cell is the primitive unit cell.

Some lattices and unit cells in two dimensions

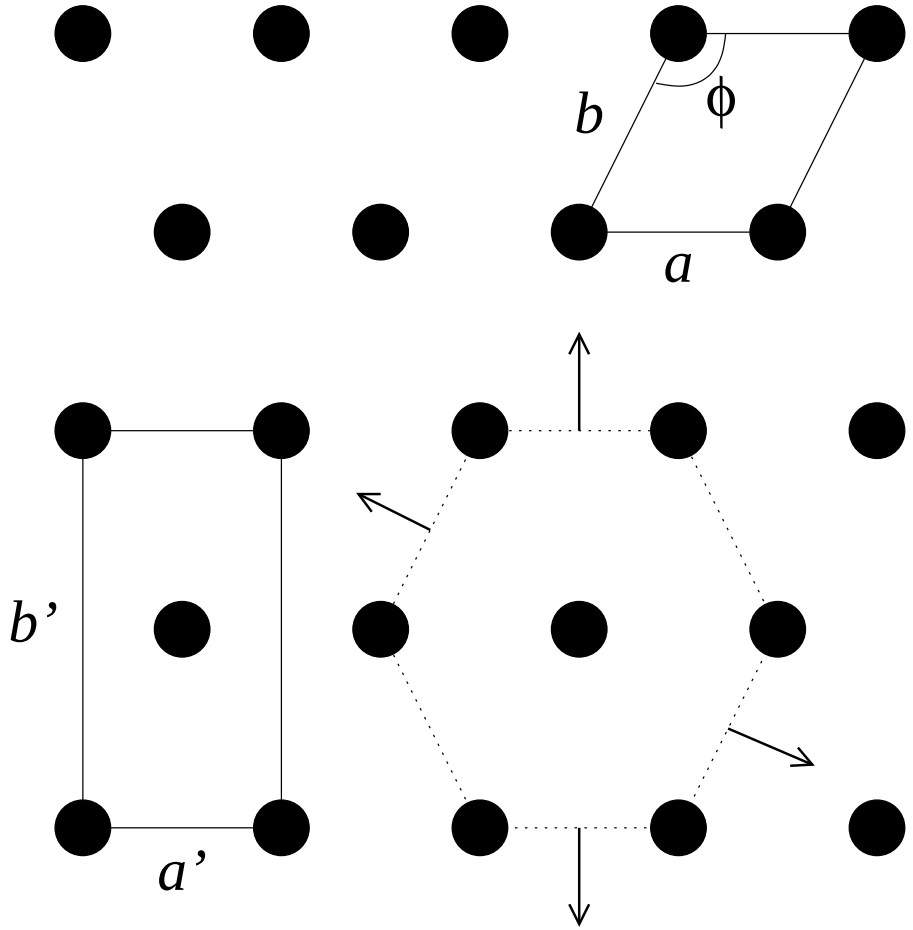
a) square



b) rectangular



c) hexagonal

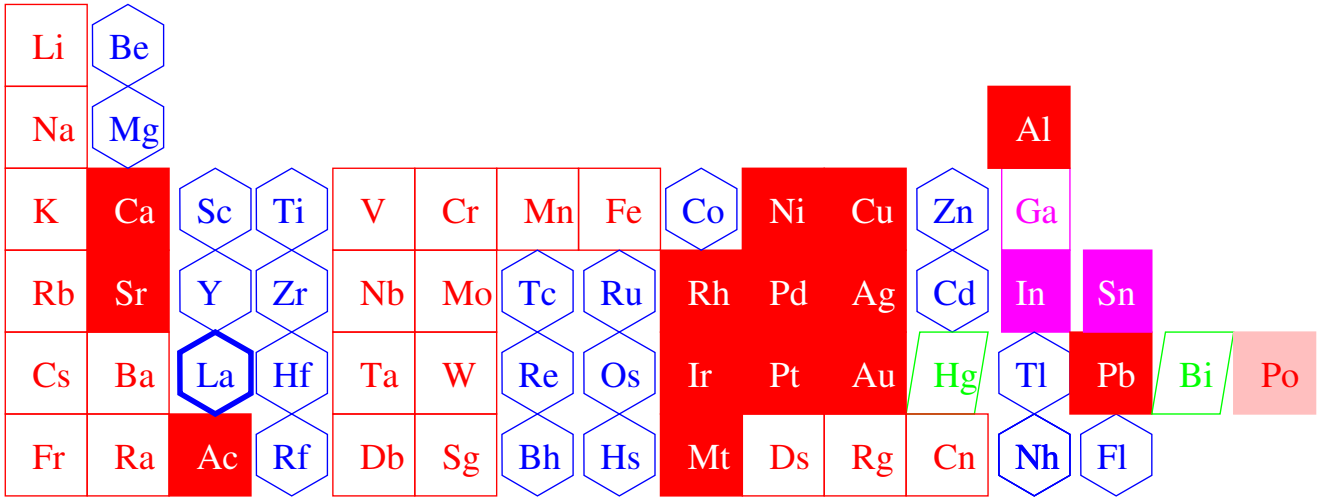


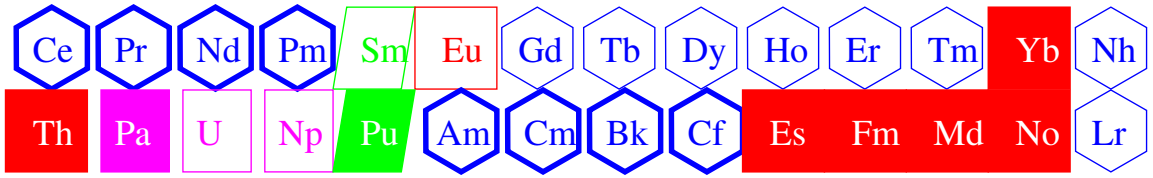
Possible crystal lattices

- In three dimensions, there are exactly 14 distinct crystal lattices known as Bravais lattices.
  `https://en.wikipedia.org/wiki/Bravais_lattice#In_3_dimensions`

Possible crystal lattices (continued)

- Almost all metals crystallize in a cubic or hexagonal lattice.





: body–centered cubic

: face–centered cubic

: simple cubic

: hexagonal close packed

: double HCP

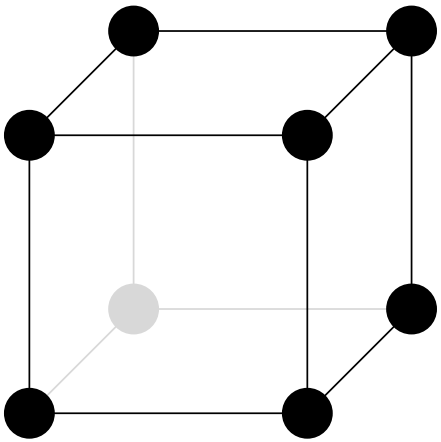
: rhombohedral

: orthorhombic

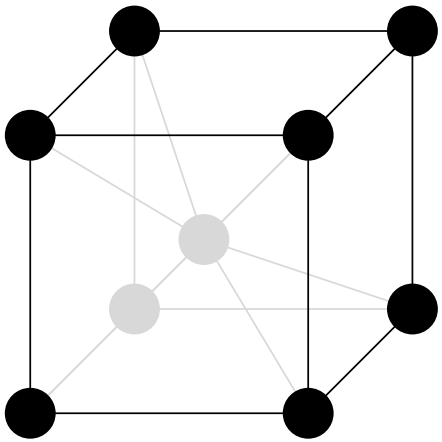
: tetragonal

: monoclinic

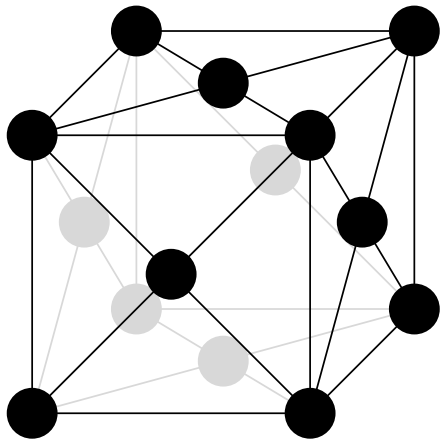
Cubic structures



simple cubic



body-centered cubic



face-centered cubic

Counting atoms in a rectangular unit cell

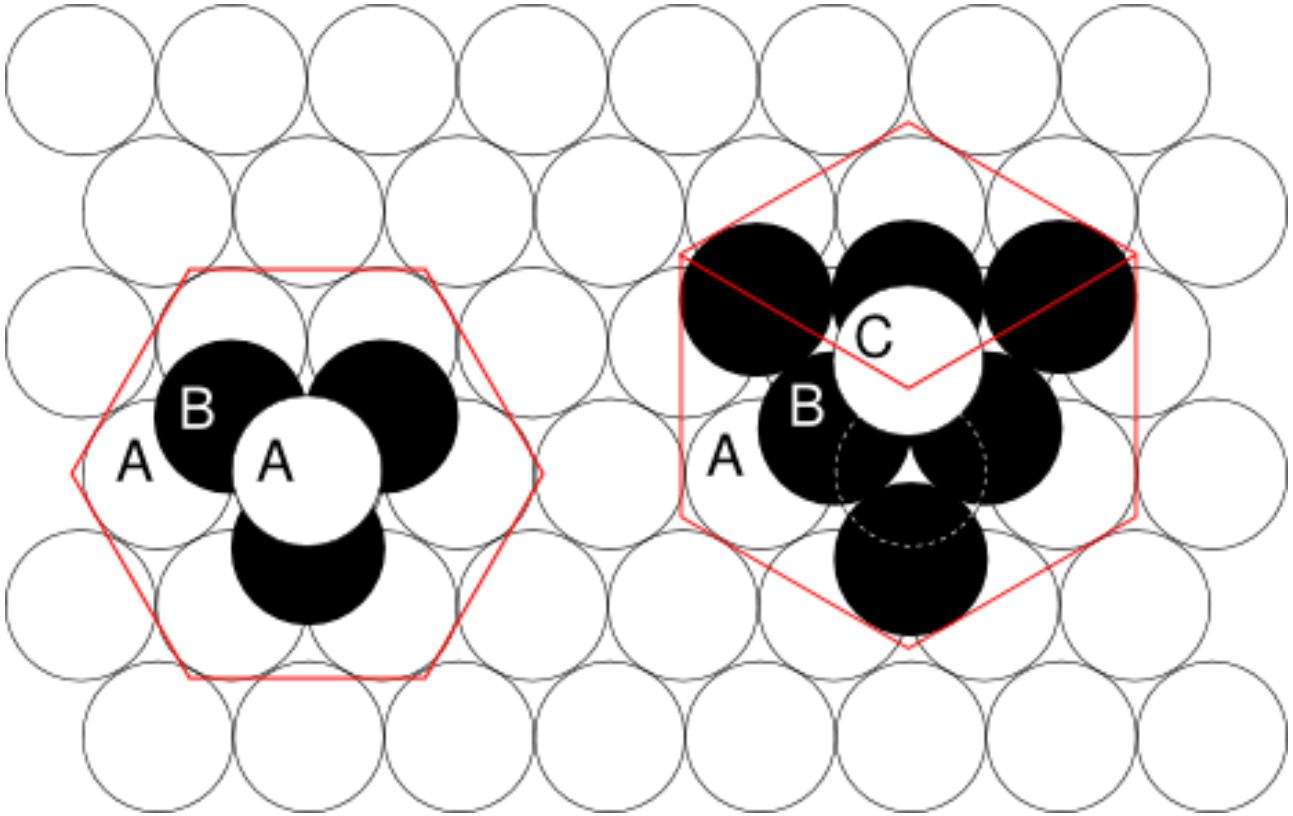
- A corner atom is shared between 8 unit cells
  $\therefore \frac{1}{8}$ of an atom is inside any given cell.
- A facial atom is shared between 2 unit cells
  $\therefore \frac{1}{2}$ of an atom is inside any given cell.
- Simple cubic: $8 \times \frac{1}{8} = 1$ atom per unit cell
- bcc: $8 \times \frac{1}{8} + 1 = 2$ atoms per unit cell
- fcc: $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$ atoms per unit cell

Closest packing

- Some structures are packed more efficiently (leave less empty space) than others.
- fcc is also known as cubic closest packed (ccp) because it has the minimum empty space.
  74% of the space is occupied by atoms.
- An identical packing fraction is obtained for the hexagonal closest packed (hcp) structure.

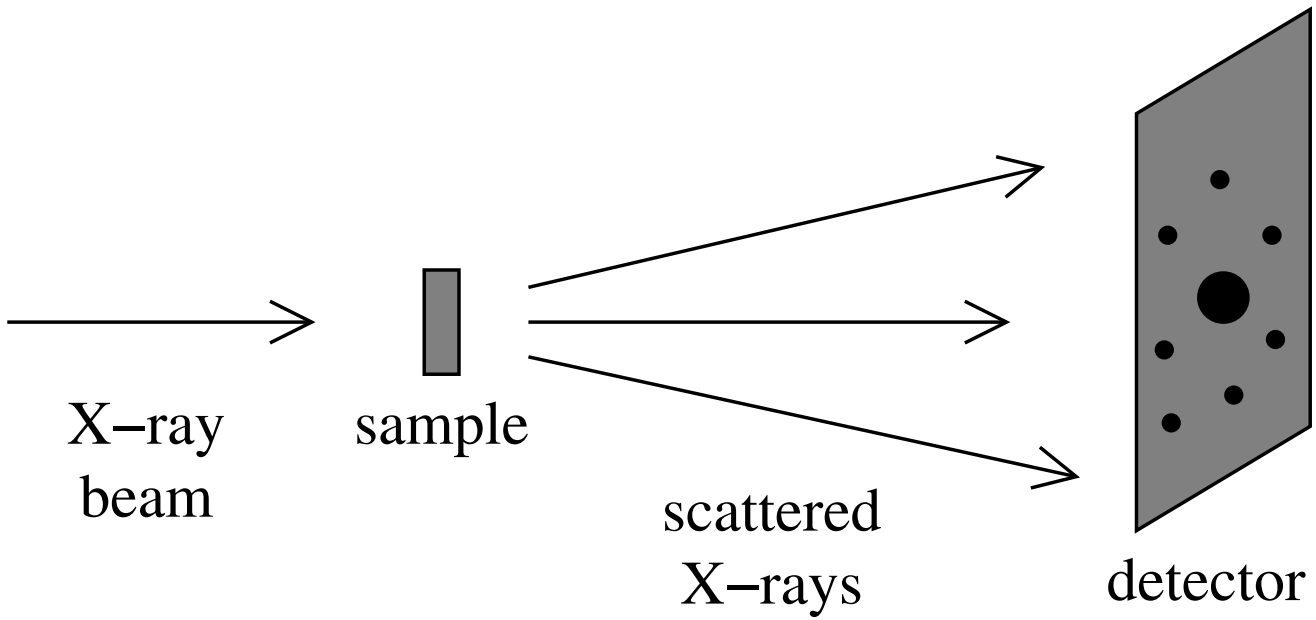
Closest packing (continued)

- hcp and fcc structures are closely related.



- hcp structure described as ABAB...
  fcc structure described as ABCABC...

X-ray diffraction



From this experiment, we get

- crystal structure (bcc, hcp, etc.)
- positions of atoms within unit cell
- dimensions of unit cell