BMM1523/BHA1113 ENGINEERING MATERIALS

STRUCTURE OF MATERIALS

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Chapter Description

- **Aims**

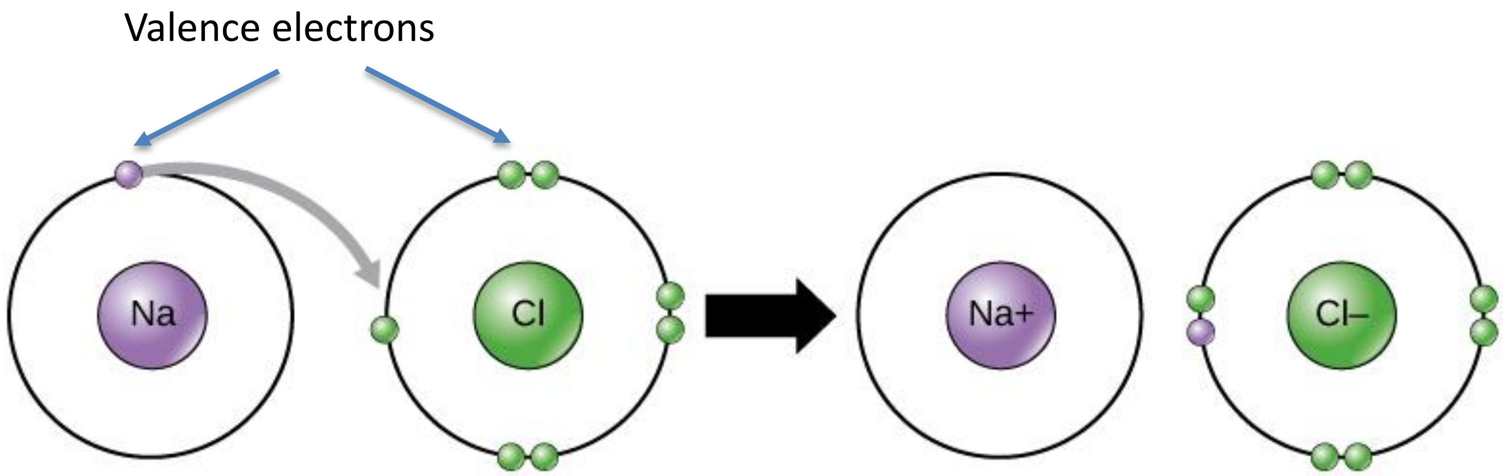
  Students are expected to have basic understanding on atomic bonding, crystal structures, and crystal defects.

- **Expected Outcomes**
  - Understand types of atomic bonding
  - Identify three common types of crystal structure in metals
  - Identify types of defect in engineering materials.

- **References**

1. William D. Callister and David G. Rethwisch. Materials science and enginnering: An Introduction, 9th Ed. Wiley, 2014.

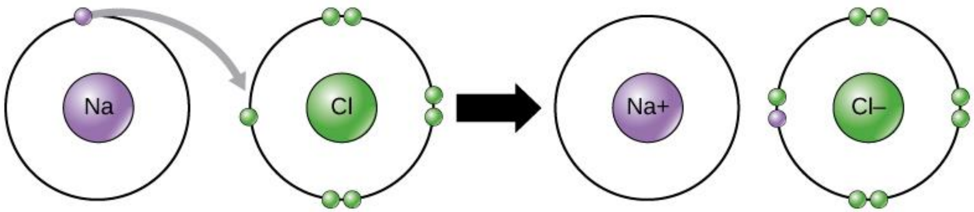
Atom and valence electrons



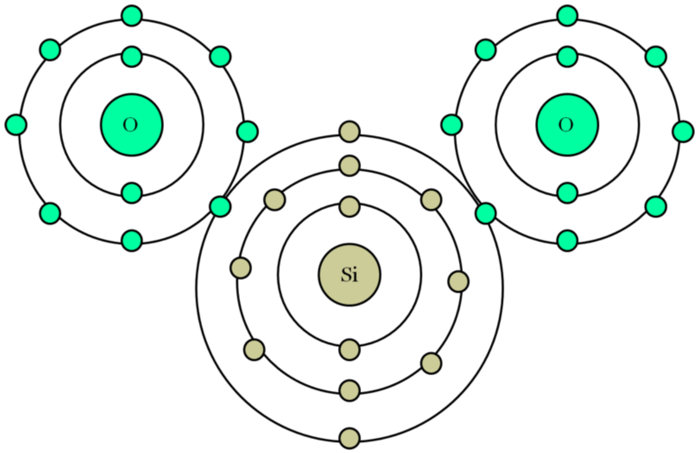
- **Valence electrons** play an important role in the bonding between atoms.
- It determine many materials properties.

Atomic bonding

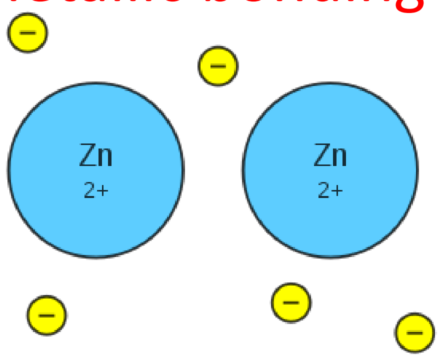
Ionic bonding



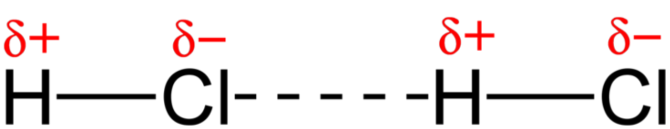
Covalent bonding



Metallic bonding



Van Der Waals bonding



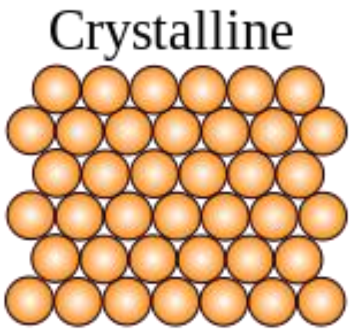
Which one produce materials with high thermal and electricity conductivity? Why?

Crystal Structures of Solid

- **Crystalline**

  Atoms arrangement in an ordered 3D pattern.

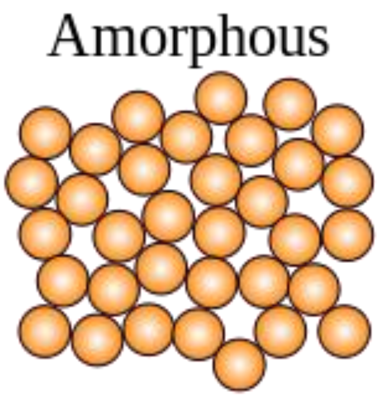
  Most metals, many ceramics and certain polymers are crystalline materials



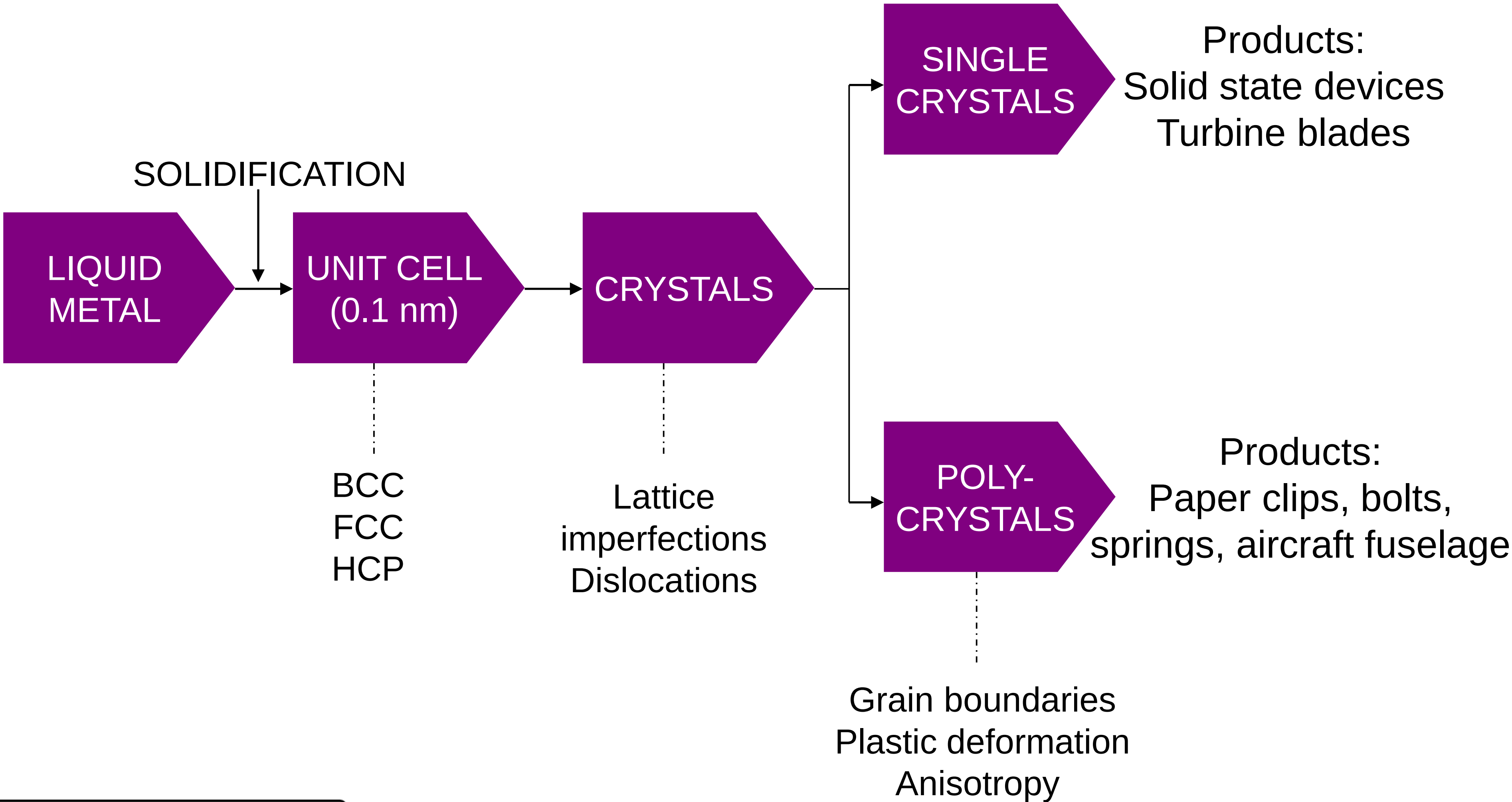
- **Amorphous**

  Atomic arrangement does not have forms. The atomic structure resemble it liquid condition.

  Glass and polymers are example of non-crystalline materials

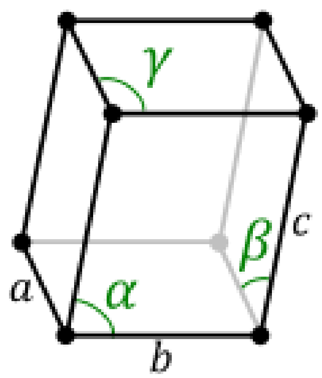


Metallic crystal structure

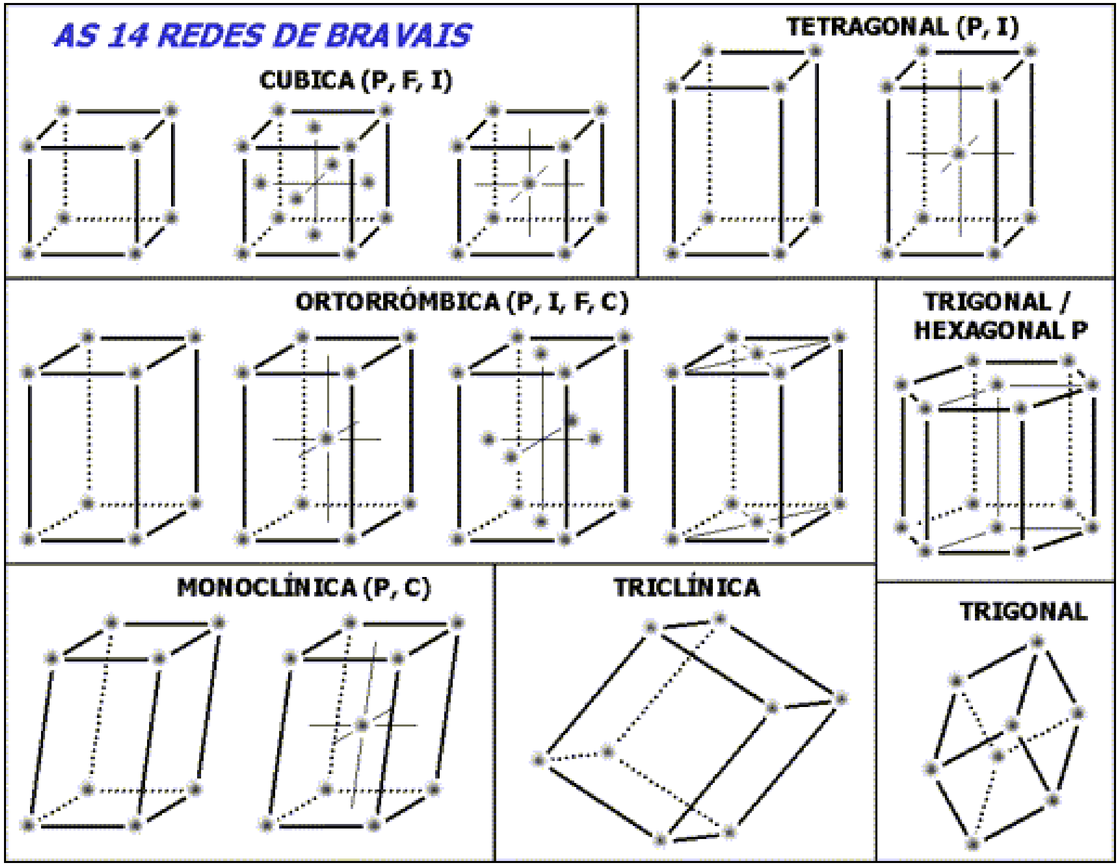


Unit Cell and Bravais Lattice

- **Unit cell: the smallest repetitive structure of crystalline materials**



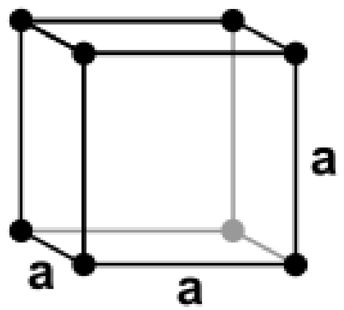
Lattice parameters



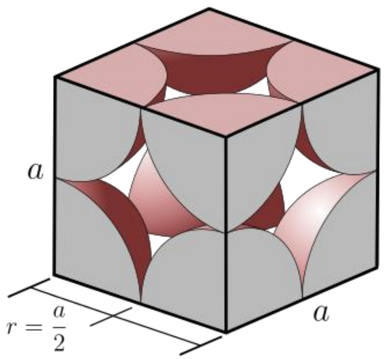
Metallic Crystal Structures
Simple Cubic (SC)

- Not common in metals due to low packing density (only Po has this structure)

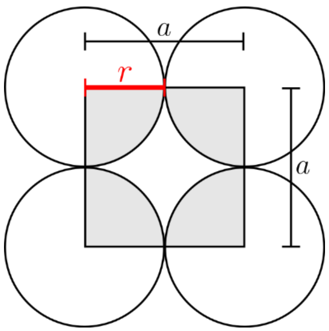
Unit cell of SC



Unit cell of SC with lattice



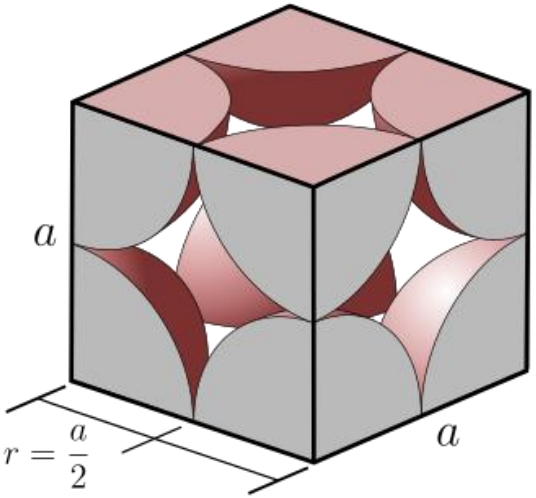
Exact parts of atoms Located in a unit cell



Relation between *a* and *r*

r = radius of atoms
a = lattice lenght

Metallic Crystal Structures
Simple Cubic (SC)



Number of atoms per unit cell, *N*

$$N = N_i + \frac{1}{2}N_f + \frac{1}{8}N_c$$

$$= 0 + \frac{1}{2}(0) + \frac{1}{8}(8) = 1\,\frac{\text{atom}}{\text{unit cell}}$$

Atomic Packing Factor (APF)

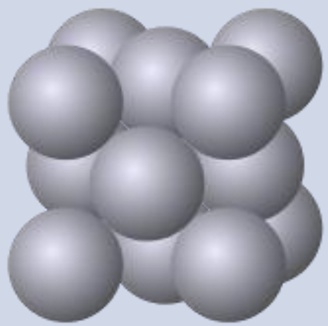
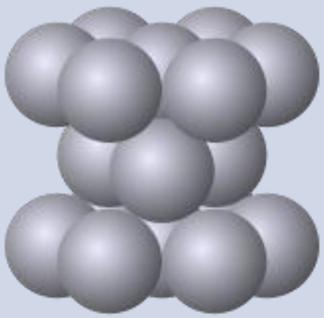
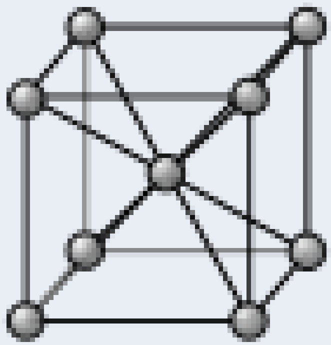
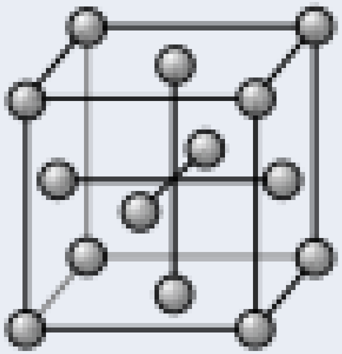
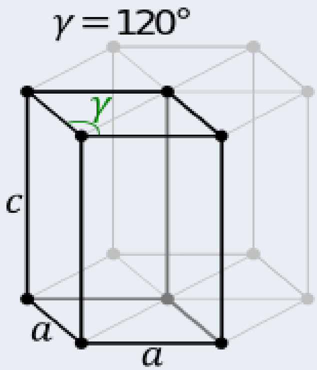
$$APF = \frac{Volume\ of\ atom\ in\ a\ unit\ cell}{Volume\ of\ unit\ cell} = \frac{N\left(\frac{4}{3}r^3\right)}{a^3}$$

$$APF = \frac{(1)\left(\frac{4}{3}r^3\right)}{(2r)^3} = 0.67\,\frac{\text{atom}}{\text{unit cell}}$$

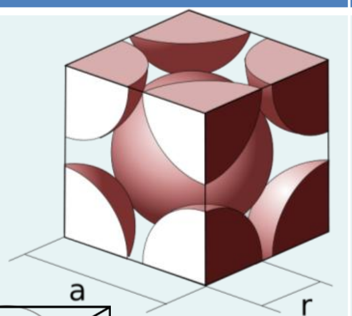
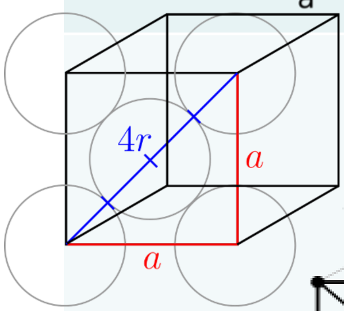
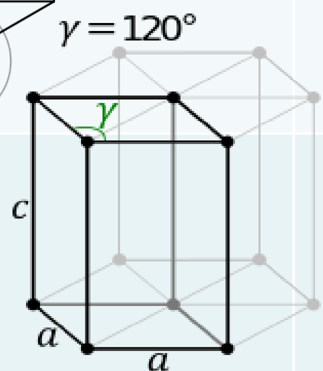
N_i = number of atoms in the center
N_f = number of atoms in the face
N_c = number of atoms in the corner

r = radius of atoms
a = lattice lenght

Metallic Crystal Structures
BCC, FCC, and HCP

Body-centered cubic (BCC)	Face-centered cubic (FCC)	Hexagonal-close packed (HCP)
		
		

Metallic Crystal Structures
BCC, FCC, and HCP

Crystal Units	Relation *a* and *r* *a* = F(*r*)	Number of atoms (*N*)	Atomic Packing Factor (APF)	Example
	**a = 4R/√3**	**2**	**0.68**	Iron (Fe) (at <910ºC),, chromium (Cr), tungsten (W), Molybdenum (Mo)
	**a = 2R√2**	**4**	**0.74**	Aluminum (Al), nickel (Ni), copper (Cu), and iron (at 912-1394ºC)
	**c/a =1.633**	**6**	**0.74**	Magnesium (Mg), zinc (Zn), cobalt (Co), zirconium (Zr), titanium (Ti),

Theoretical Density, ρ

$$\rho = \frac{Mass\ of\ atoms\ in\ unit\ cell}{Total\ volume\ of\ unit\ cell}$$

$$\rho = \frac{N\ A}{V\ N_A}$$

N = Number of atoms in a unit cell, atoms/unitcell
A = Atomic weight, g/mol
V = volume of unit cell, cm^3
N_A = Avogadro's number, 6.022×10^{23} atom/mol

Try this:

Calculate the theoretical density of Chromium (Cr), if the atom has BCC crystal structure with atomic radius of 0.125 nm and molecular weight of 52.00 g/mol. (Answer = 7.18 g/cm^3)

Densities of Material Classes

In general

$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$

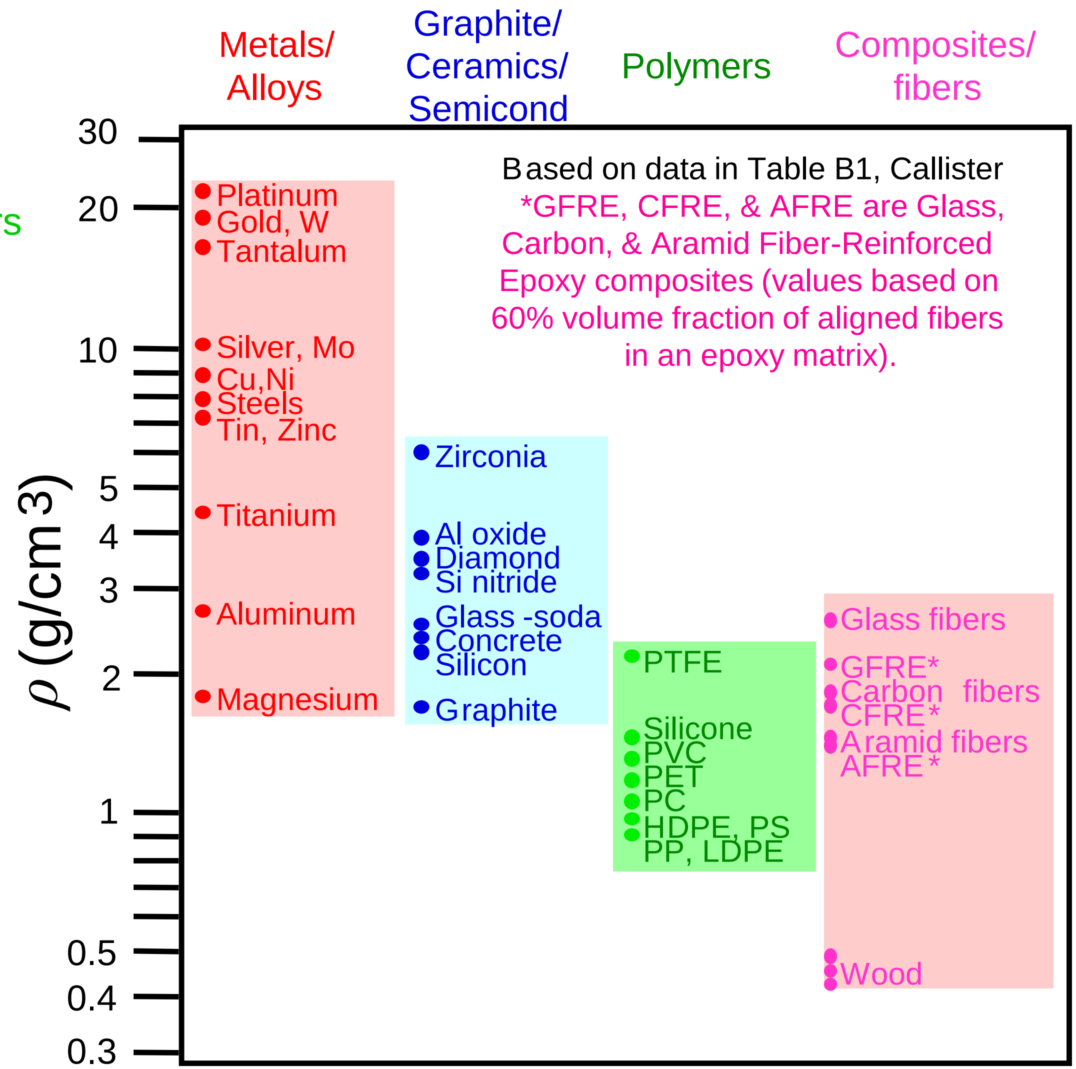
Why?

Metals have...
- close-packing (metallic bonding)
- often large atomic masses

Ceramics have...
- less dense packing
- often lighter elements

Polymers have...
- low packing density (often amorphous)
- lighter elements (C,H,O)

Composites have...
- intermediate values



Data from Table B.1, *Callister & Rethwisch, 9e.*

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Research Interest:

- ❑High Temperature Physical Chemistry
- ❑Thin Films Technology
- ❑Metals and Alloys.

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