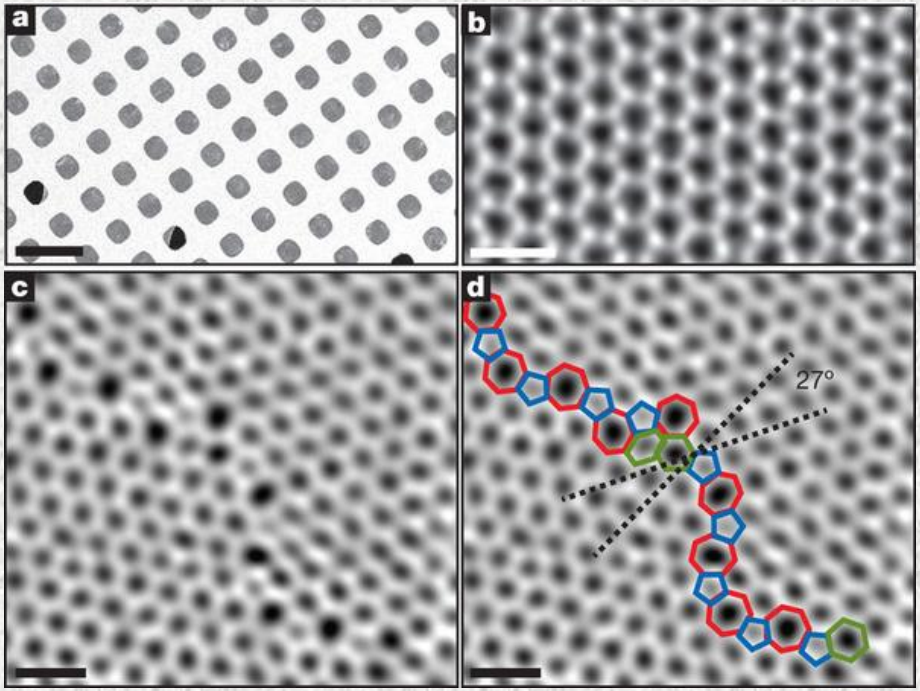
Defect in crystals



Primer Materials For Science Teaching

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Introduction

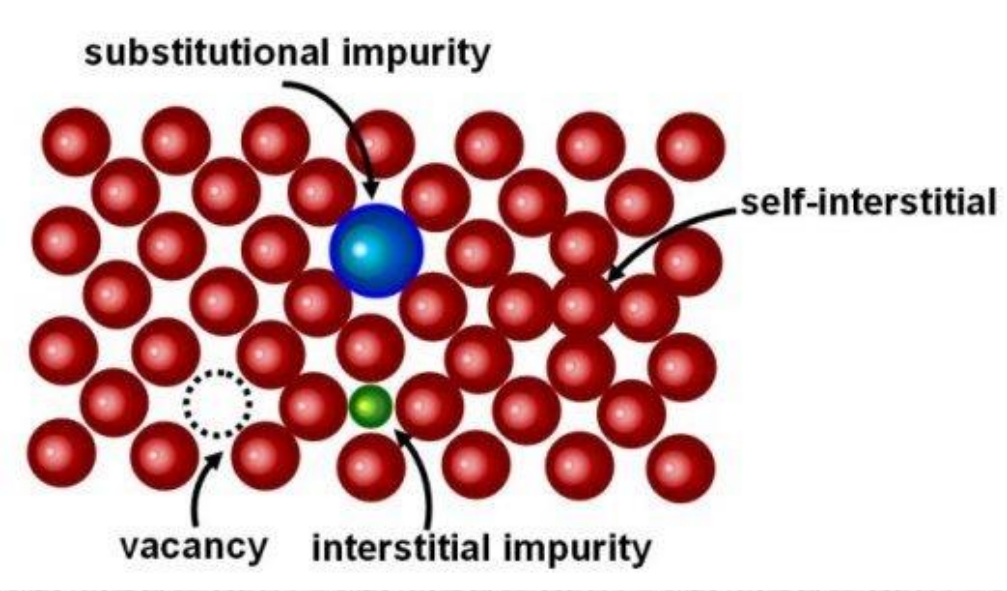
- The arrangement of the atoms in all materials contains imperfections which have profound effect on the behavior of the materials
- Lattice defects can be sorted into three
  1. Point defects (vacancies, interstitial defects, substitution defects)
  2. Line defect (screw dislocation, edge dislocation)
  3. surface defects (material surface, grain boundaries)

Why defect are important?

There are a lot of properties that are controlled or affected by defects, for example:

- Electric and thermal conductivity in metals (strongly reduced by point defects).
- Electronic conductivity in semi-conductors (controlled by substitution defects).
- Diffusion (controlled by vacancies).
- Ionic conductivity (controlled by vacancies).
- Plastic deformation in crystalline materials (controlled by dislocation).
- Colors (affected by defects).
- Mechanical strength (strongly depended on defects).

Points defects



Self-interstitial – A self-interstitial is an atom from the crystal that is crowded into an interstitial site, a small void space that under ordinary circumstances is not occupied.
the formation of this defect is not highly probable, and it exists in very small concentrations

Vacancies

- A **vacancy** is produced when an atom is missing from a normal site.
- The equilibrium number of vacancies Nv has Temp depends:
  - N – Total number of atoms
  - Qv – energy require for vacancy formation

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

Example 3.1

Calculate the equilibrium value of vacancies concentration for copper at 1000K. the energy for vacancy formation is 0.9 eV/atom;

$Qv := 0.9\,eV$ $\quad KB := 1.38 \cdot 10^{-23}\,\frac{J}{K}$ $\quad T := 1000K$

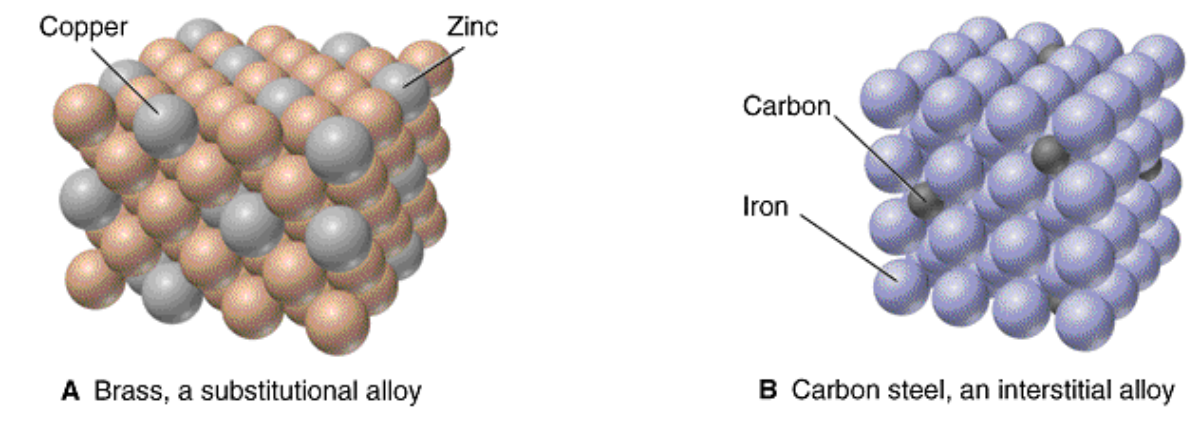
$1eV = 1.602 \times 10^{-19}\,J$

$$e^{\frac{-Qv}{KB \cdot T}} = 2.939 \times 10^{-5}$$

One vacancy per $\frac{1}{(2.939 \times 10^{-5})} = 3.403 \times 10^{4}$ copper atoms

Impurities in solids

- A pure metal consisting of only one type of atom just isn't possible.
- impurity or foreign atoms will always be present, and some will exist as crystalline point defects.
- The addition of impurity atoms to a metal will result in the formation of a solid solution



- Impurity point defects are found in solid solutions, of which there are two types:
  1. Substitutional – one atom is replaced by as different type of atom
  2. Interstitial – extra atom is inserted into the lattice structure at a normally unoccupied position

Hume-Rothery rules

For the substitutional type there are several features of the solute and solvent atoms that determine the degree to which the former dissolves in the latter, as follows:

1. ***Atomic size factor –*** The atomic radii of the solute and solvent atoms must differ by no more than 15%

2. ***Crystal structure -*** The crystal structures of solute and solvent must match.

3. ***Electronegativity -*** The solute and solvent should have similar electronegativity. If the electronegativity difference is too great, the metals will tend to form intermetallic compounds instead of solid solutions.

4. ***Valences -*** Complete solubility occurs when the solvent and solute have the same valency. A metal will have more of a tendency to dissolve another metal of higher valence than one of a lower valence

Example 3.2

Using Hume-Rothery rule please predict whether these metals will or will not be soluble in each other

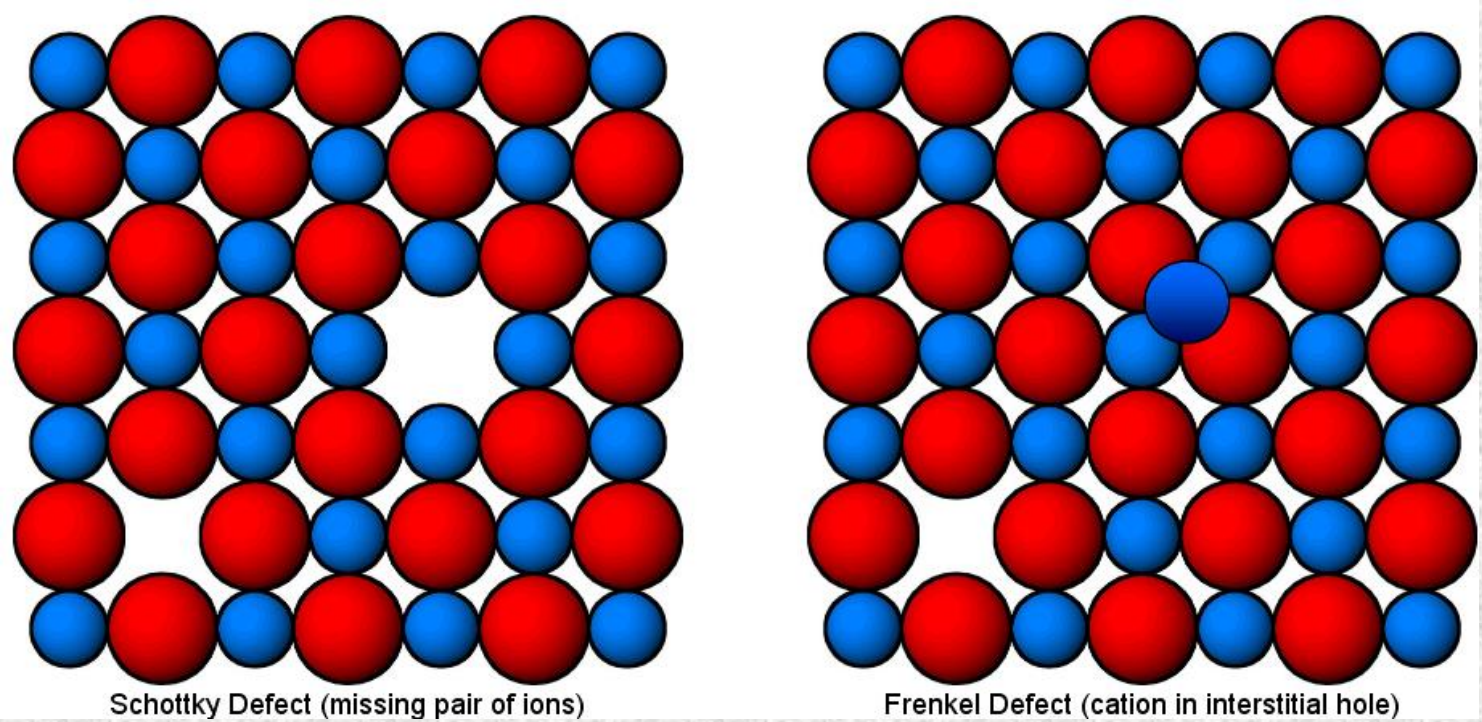
a) Fe and Cu. r_{Cu}=0.128nm, r_{Fe}=0.126 nm; Fe=BCC, Cu=FCC; Cu^{+}/ Cu^{+2}, Fe^{3+}/ Fe^{+2}
- No soluble at room temperature, slightly soluble at high temperature

b) Ni and Cu. r_{Cu}=0.128nm, r_{Ni}=0.125 nm; Ni=FCC, Cu=FCC; Ni^{+2}, Cu^{+}/ Cu^{+2}
- fully soluble

c) Al and Ag. r_{Al}=0.143nm, r_{Ag}=0.144 nm, Al=FCC, Cu=FCC; Al^{+3}, Ag^{+1}
- Al is soluble of in Ag, Ag is slightly soluble in Al.

Other points defects

- **Frenkel defect** – ion jumps from a normal lattice point to an interstitial site, leaving behind a vacancy (vacancy-interstitial)
- **Schottky** – pair of vacancies in ionically bonded material. Both anion and cation must be missing from the lattice to maintain the crystal neutral.

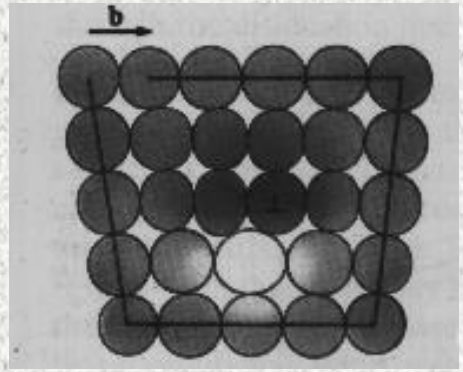


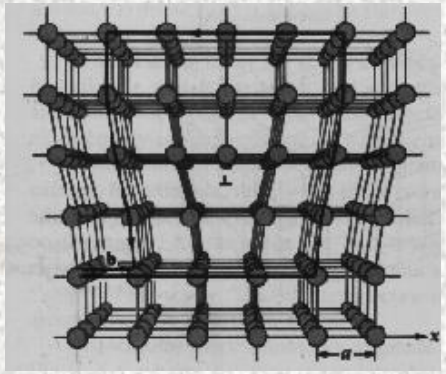
Schottky Defect (missing pair of ions)

Frenkel Defect (cation in interstitial hole)

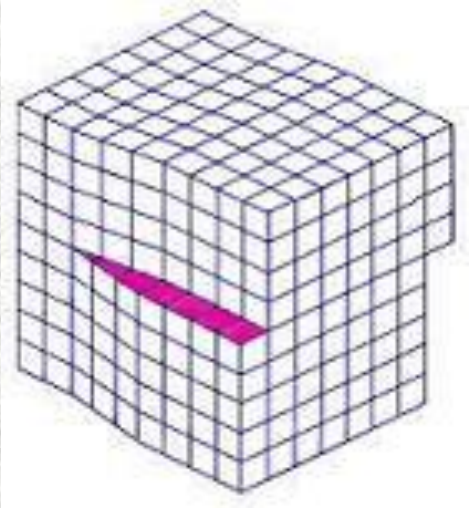
Line defects - Dislocations

Edge Dislocation





Screw Dislocation



Dislocation movement