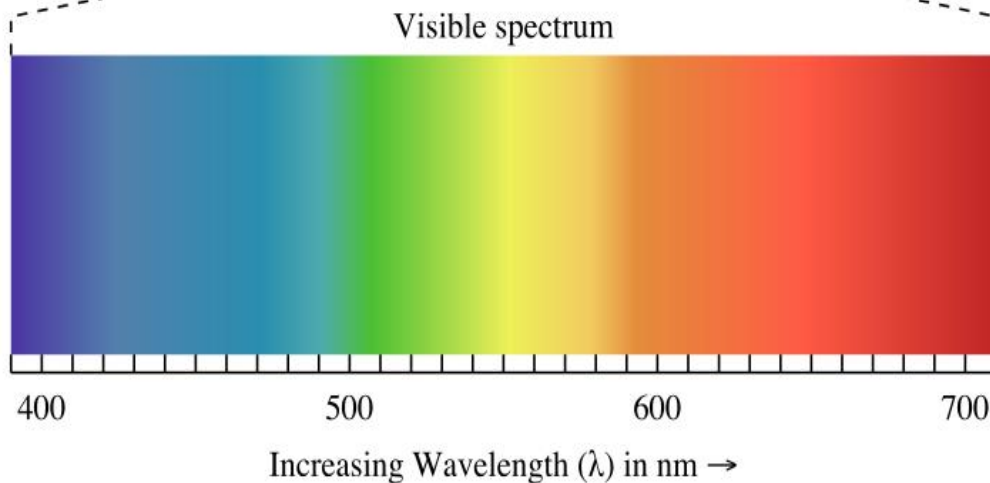
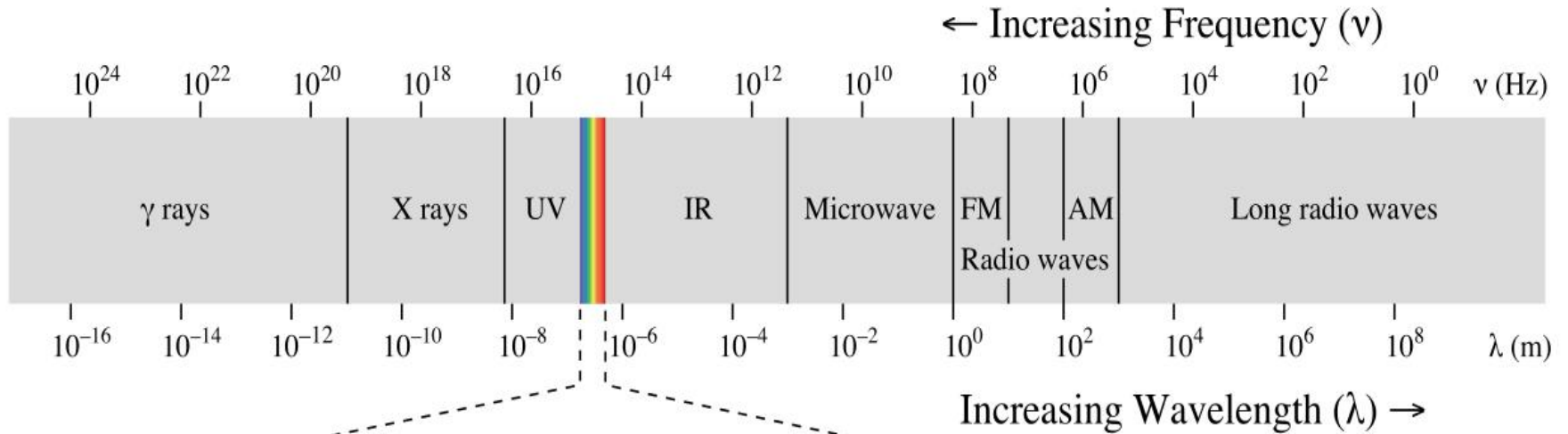


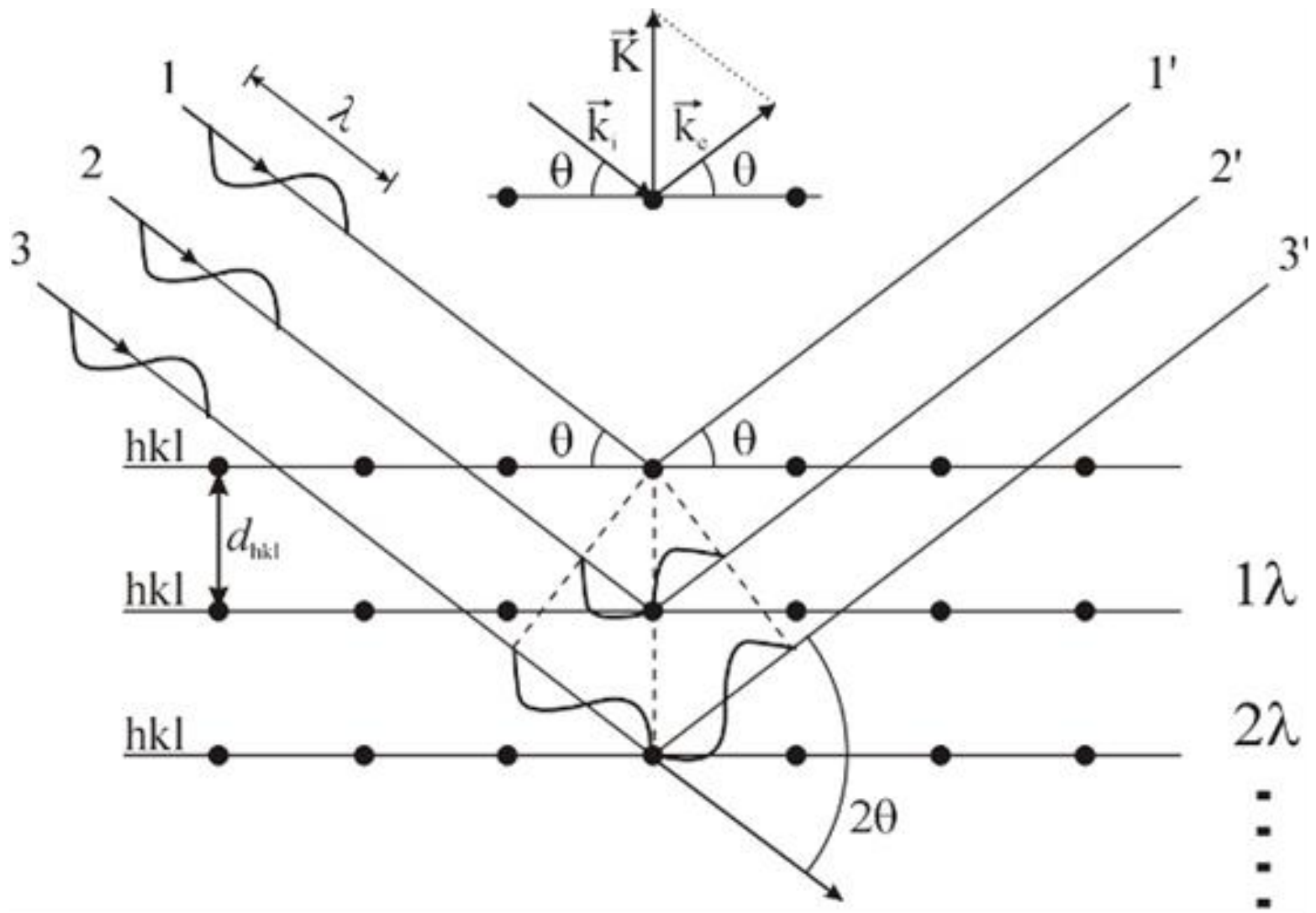
X-Ray Diffraction



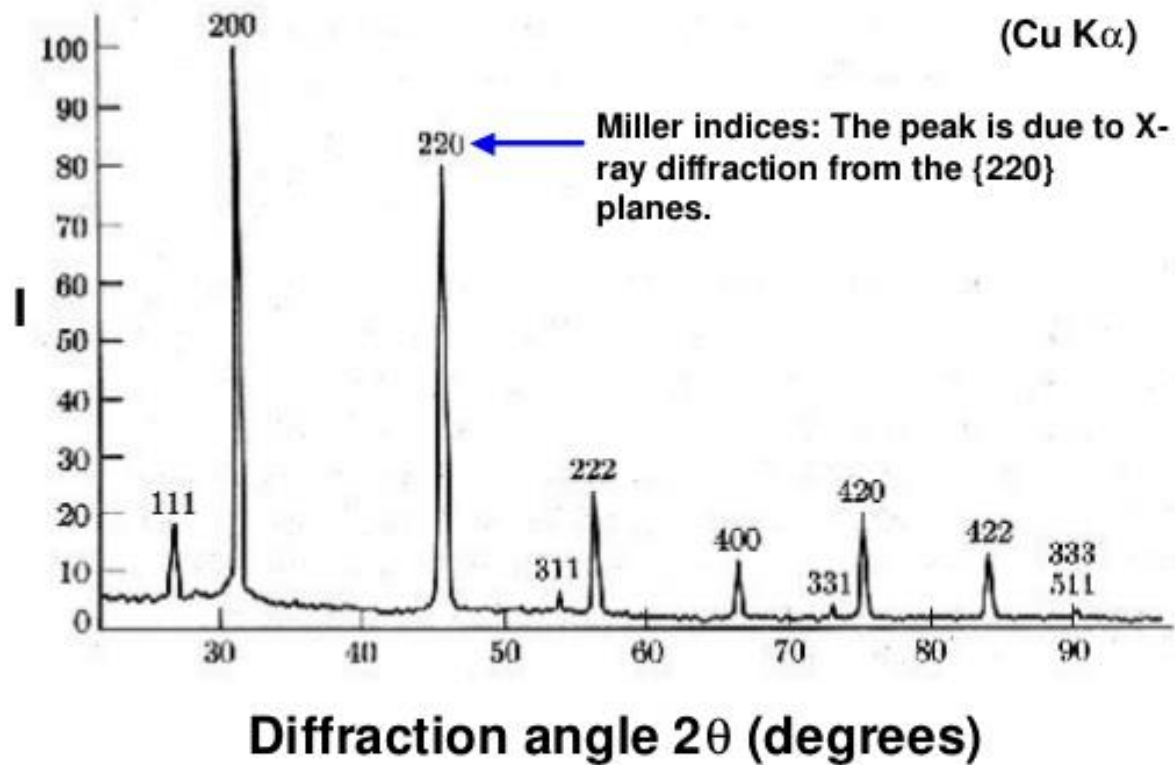
Bragg's Law : $n\lambda=2d\sin\theta$

Electromagnetic Spectrum





XRD Pattern of NaCl Powder



Orthorhombic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Tetragonal

$$\frac{1}{d_{hkl}^2} = \left[h^2 + k^2 + l^2 \left(\frac{a}{c} \right)^2 \right] \frac{1}{a^2}$$

Cubic

$$\frac{1}{d_{hkl}^2} = (h^2 + k^2 + l^2) \frac{1}{a^2}$$

Monoclinic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2 \sin^2 \gamma} + \frac{k^2}{b^2 \sin^2 \gamma} - \frac{2hk \cos \gamma}{ab \sin^2 \gamma} + \frac{l^2}{c^2}$$

Hexagonal

$$\frac{1}{d_{hkl}^2} = \left[\frac{4}{3} (h^2 + k^2 + hk) + l^2 \left(\frac{a}{c} \right)^2 \right] \frac{1}{a^2}$$

Triclinic

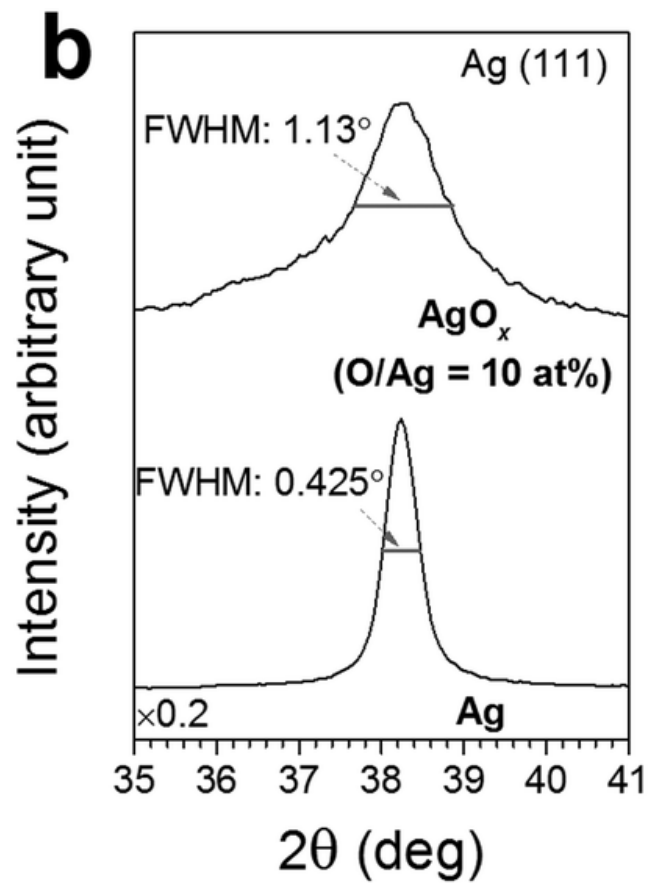
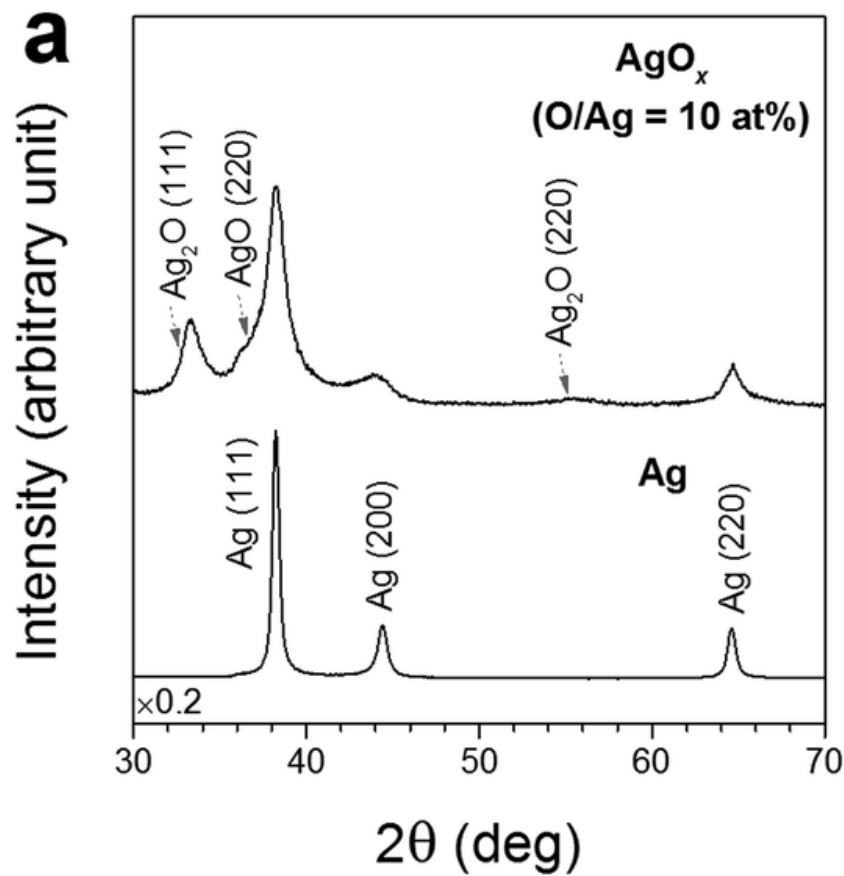
$$\frac{1}{d_{hkl}^2} = \begin{bmatrix} \frac{h}{a} \cos \gamma \cos \beta \\ \frac{h}{a} \frac{k}{b} \cos \alpha \\ \frac{l}{c} \cos \alpha \end{bmatrix} + \frac{k}{b} \begin{bmatrix} 1 \frac{h}{a} \cos \alpha \\ \cos \gamma \frac{k}{b} \cos \alpha \\ \cos \beta \frac{l}{c} \end{bmatrix} + \frac{l}{c} \begin{bmatrix} 1 \cos \gamma \frac{h}{a} \\ \cos \gamma \cos \alpha \frac{k}{b} \\ \cos \beta \cos \alpha \frac{l}{c} \end{bmatrix} \cdot \begin{bmatrix} 1 \cos \gamma \cos \beta \\ \cos \gamma \cos \alpha \\ \cos \beta \cos \alpha \end{bmatrix}^{-1}$$

Trigonal (rhombohedral)

$$\frac{1}{d_{hkl}^2} = \frac{[(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + lh) (\cos^2 \alpha - \cos \alpha)]}{A^2 (1 + 2 \cos^3 \alpha - 3 \cos^2 \alpha)}$$

Sherrer Equation (useful for crystals/powders less than 100 nm)

$$t = \frac{0.9\lambda}{B_{\text{size}} \cos \theta_B}$$



List of selection rules for different crystals

Crystal Type	Bravais Lattice	Reflections Present	Reflections Absent
Simple	Primitive, P	Any h, k, l	None
Body-centered	Body centered, I	$h+k+l = \text{even}$	$h+k+l = \text{odd}$
Face-centered	Face-centered, F	h, k, l unmixed	h, k, l mixed
NaCl	FCC	h, k, l unmixed	h, k, l mixed
Zincblende	FCC	Same as FCC, but if all even and $h+k+l \neq 4N$ then absent	h, k, l mixed and if all even and $h+k+l \neq 4N$ then absent
Base-centered	Base-centered	h, k both even or both odd	h, k mixed
Hexagonal close-packed	Hexagonal	$h+2k=3N$ with l even $h+2k=3N \pm 1$ with l odd $h+2k=3N \pm 1$ with l even	$h+2k=3N$ with l odd

DEFECTS

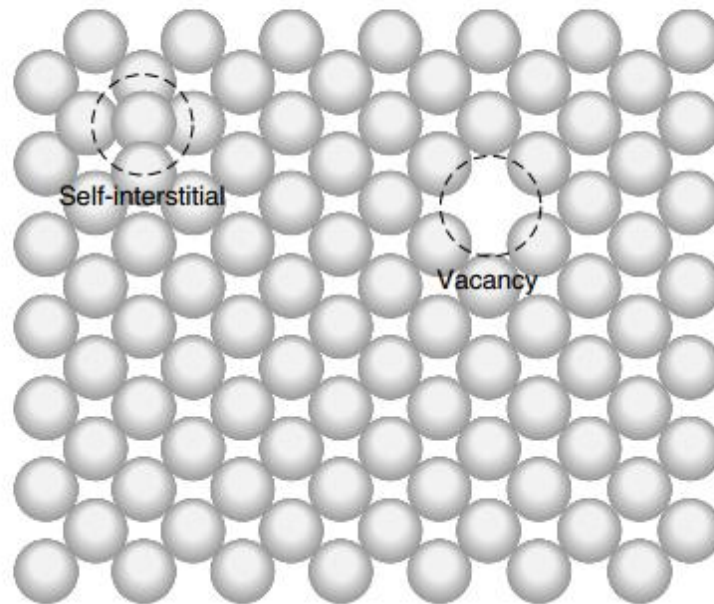
Now that the most important aspects of perfect crystals have been described, it is time to recognize that things are not always perfect, even in the world of space lattices. This is not necessarily a bad thing. As we will see, many important materials phenomena that are based on defective structures can be exploited for very important uses. These defects, also known as imperfections, are grouped according to spatial extent.

Point defects have zero dimensions; *line defects*, also known as dislocations, are one dimensional; and *planar defect* such as surface defects and grain boundary defects have two dimensions. These defects may occur individually or in combination.

Let us first examine what happens to a crystal when we remove, add, or displace an atom in the lattice. We will then describe how a different atom, called an impurity (regardless of whether or not it is beneficial), can fit into an established lattice.

POINT DEFECTS

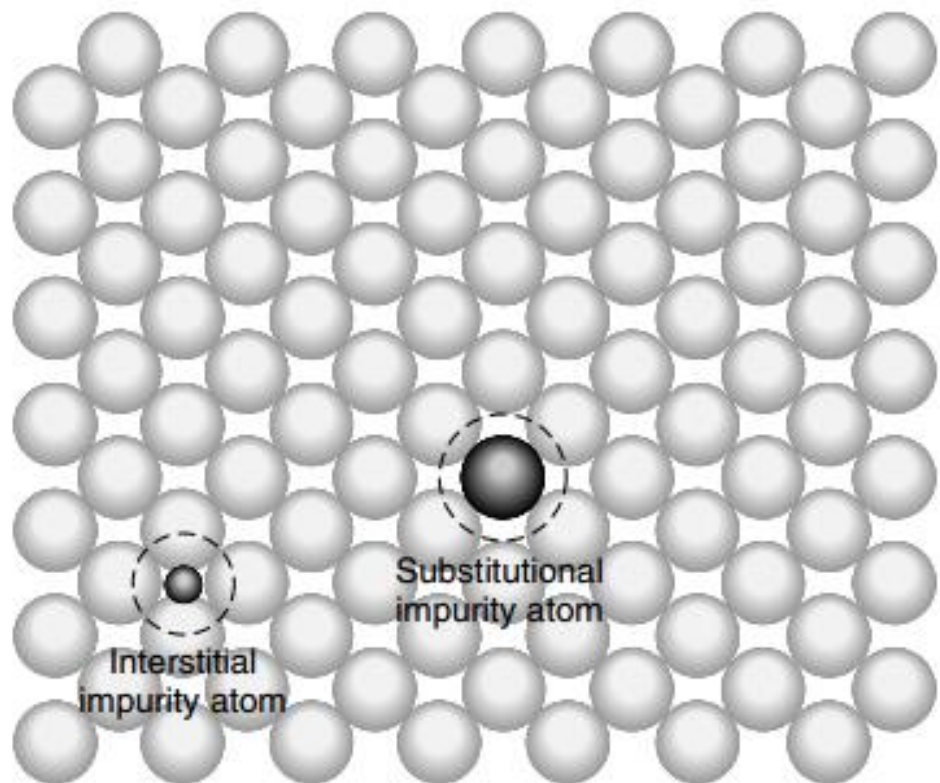
Vacancies, self-interstitials, impurity interstitials, substitutional impurities



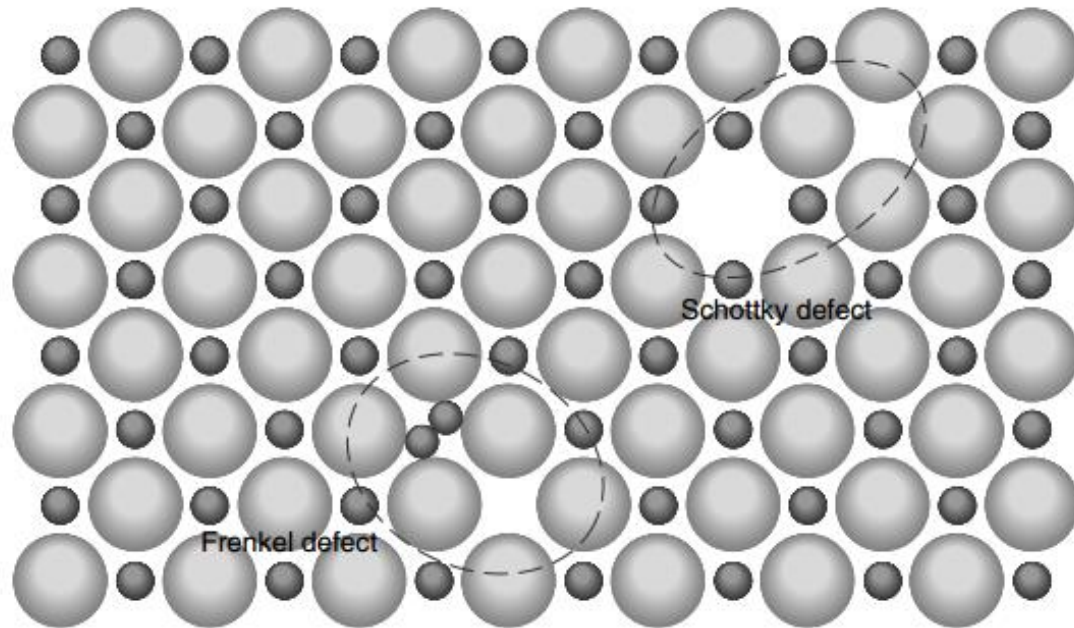
$$N_d = N \exp\left(-E_d / k_B T\right)$$

N_d is the equilibrium number of point defects, N is the total number of atomic sites per volume or mole, E_d is the activation energy for formation of the defect, k_B is Boltzmann's constant (1.38×10^{-23} J/atom · K), and T is absolute temperature in K.

Element	E_d (kJ/mol)	Melting Point, T_m (°C)	N_d (vacancies/cm ³)			
			25°C	300°C	600°C	T_m
Ag	106.1	960	1.5×10^4	1.5×10^{13}	3.0×10^{16}	7.8×10^{17}
Al	73.3	660	1.0×10^{10}	1.2×10^{16}	2.4×10^{18}	5.0×10^{18}
Au	94.5	1063	1.5×10^6	1.5×10^{14}	1.5×10^{17}	1.2×10^{19}
Cu	96.4	1083	1.1×10^6	1.4×10^{14}	1.4×10^{17}	9.0×10^{18}
Ge	192.9	958	<1	1.3×10^5	1.3×10^{11}	8.2×10^{13}
K	38.6	63	2.1×10^{15}	—	—	1.3×10^{16}
Li	39.5	186	4.7×10^{15}	—	—	1.4×10^{18}
Mg	85.8	650	4.4×10^7	6.4×10^{14}	3.5×10^{17}	5.7×10^{17}
Na	38.6	98	4.0×10^{15}	—	—	1.0×10^{17}
Pt	125.4	1769	8.7	2.7×10^{11}	2.0×10^{15}	4.2×10^{19}
Si	221.8	1412	<1	3.1×10^2	2.5×10^9	8.0×10^{15}



Point Defects in Ionic Crystals



Vacancy – increase in diffusion (next chapter), increase in ionic conductivity in some crystals, the concentration of vacancies changes with temperature (it is possible to increase vacancy concentration by playing with kinetics (next chapter))

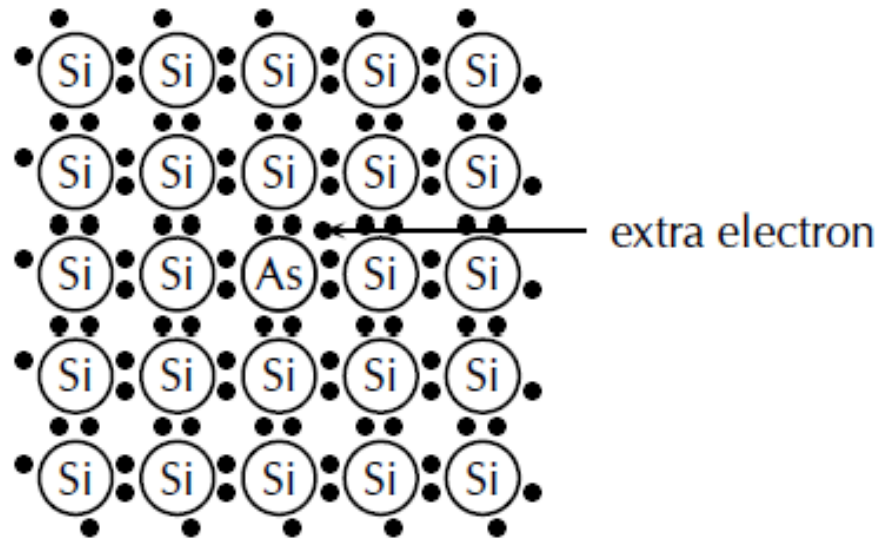
Impurity size usually dictates the defect type; substitutional or interstitial

Point defects (usually substitutional impurities) in covalent materials, especially in

semiconductors add unique properties to the material. Like As (V) in Si (IV) \rightarrow 1 free

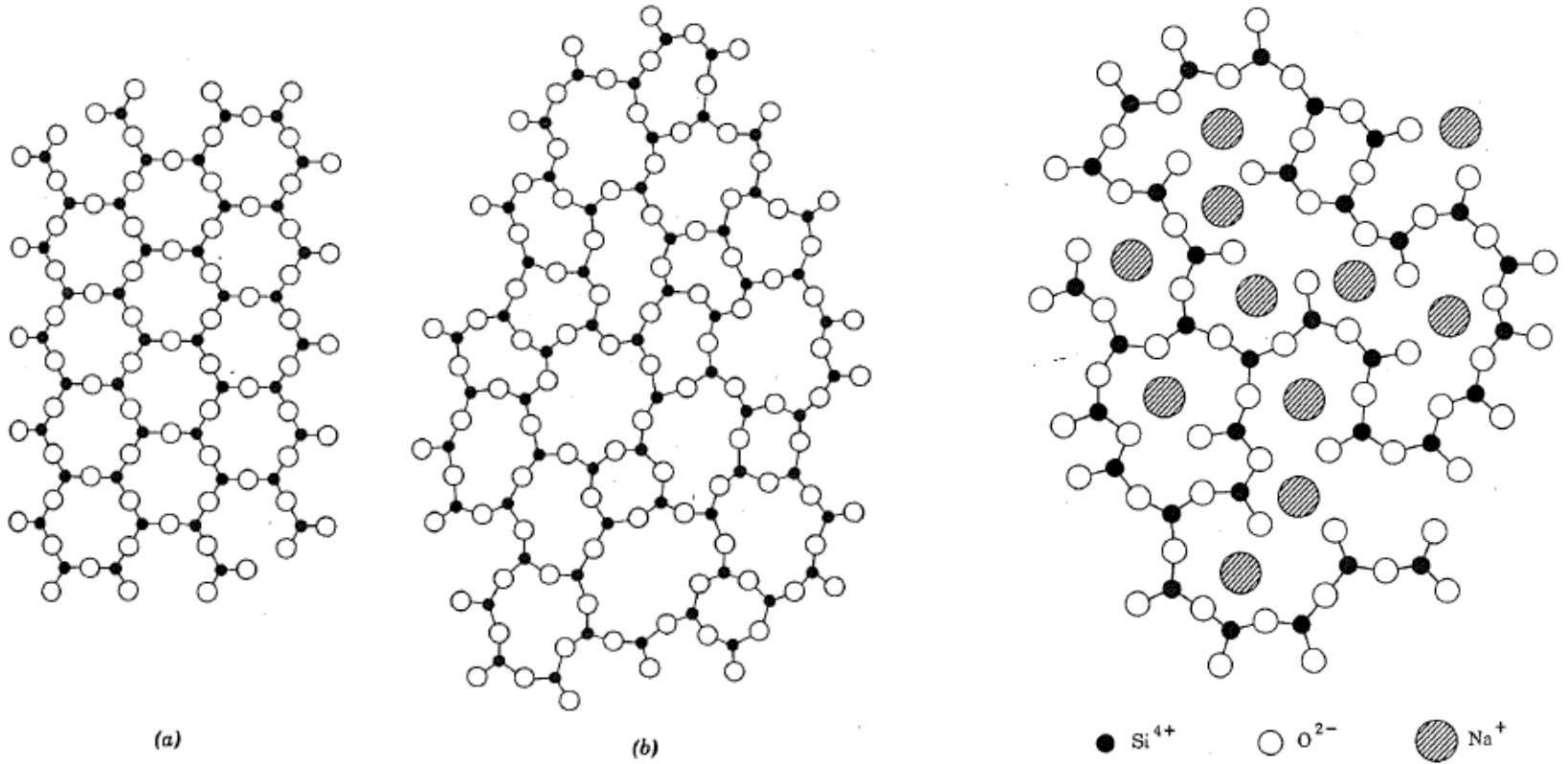
electron from As \rightarrow electrical conductivity of Si increases with increasing concentration of

As.



Impurity atoms in amorphous structure

In silica glass – network modifiers (alkali and earth alkali oxides) go into gaps and break bridging Si-O-Si bonds → lowers melting point



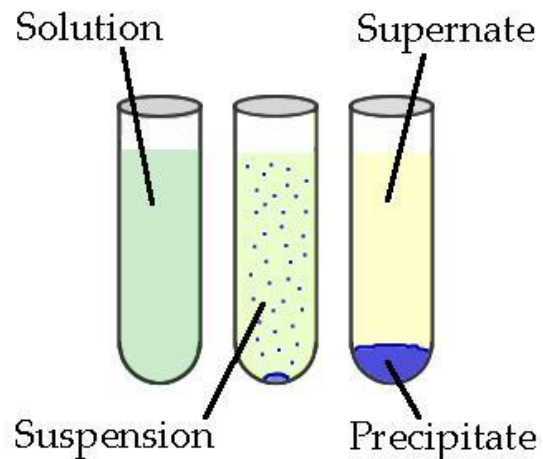
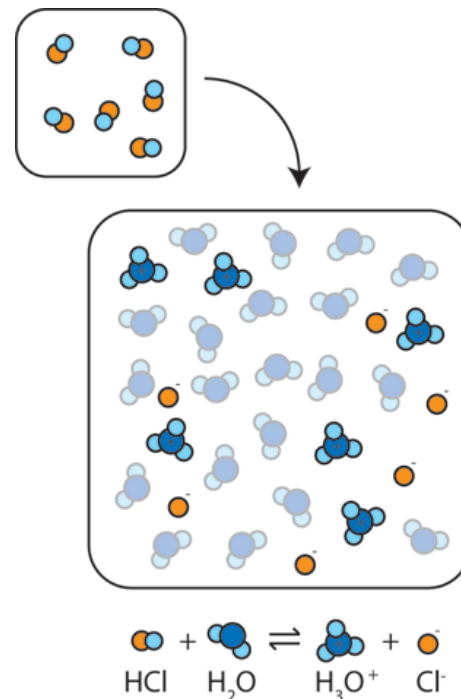
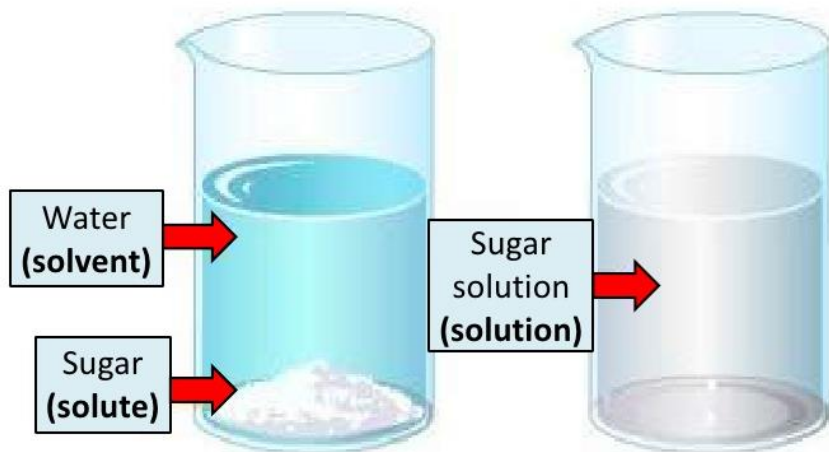
Schematic representation of (a) ordered crystalline form and (b) random-network glassy form of the same composition.

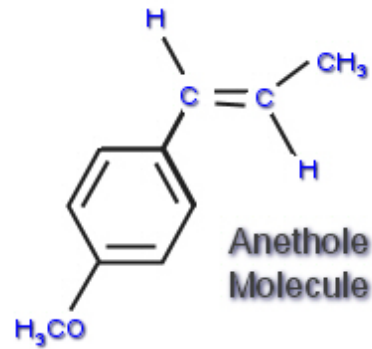
Schematic representation of the structure of a sodium silicate glass.

The concept of Solid Solution

Chemical Solution

A solution is a mixture formed when one or more solutes dissolve in a solvent.





Anethole

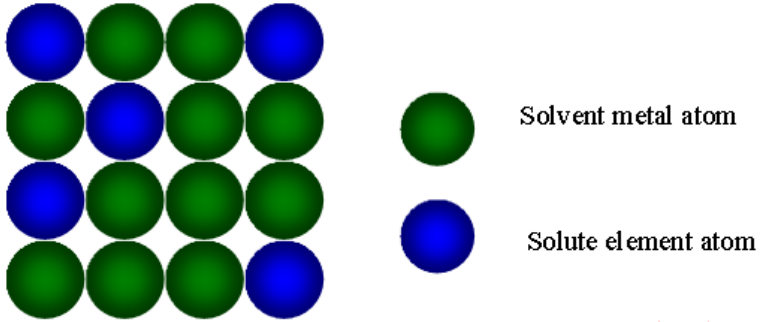
From Wikipedia, the free encyclopedia

Anethole (anise camphor) is an organic compound that is widely used as a **flavoring** substance. It is a derivative of **phenylpropene**, a type of aromatic compound that occurs widely in nature, in **essential oils**. It contributes a large component of the odor and flavor of **anise** and **fennel** (both in the botanical family **Apiaceae**), **anise myrtle** (**Myrtaceae**), **liquorice** (**Fabaceae**), **camphor**, **magnolia blossoms**, and **star anise** (**Illiciaceae**). Closely related to anethole is its isomer **estragole**, abundant in **tarragon** (**Asteraceae**) and **basil** (**Lamiaceae**), that has a flavor reminiscent of anise. It is a colorless, fragrant, mildly volatile liquid.^[1] **Anethole is only slightly soluble in water but exhibits high solubility in ethanol. This difference causes certain anise-flavored liqueurs to become opaque when diluted with water, the ouzo effect.**

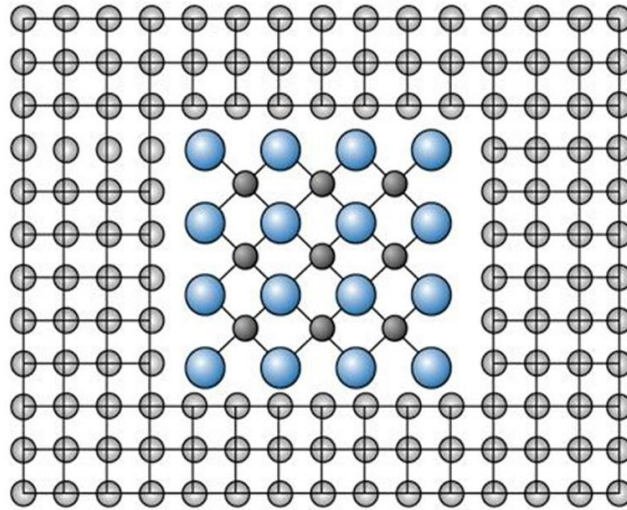
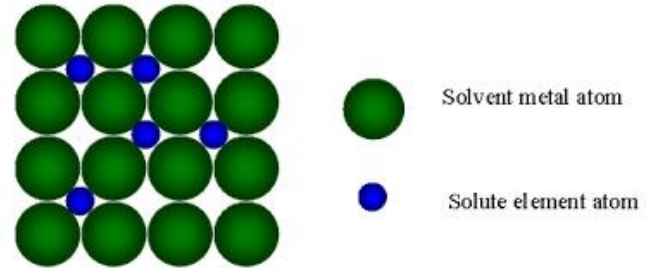


The concept of Solid Solution

Substitution solid solution



Interstitial solid solution



Hume - Rothery Rules

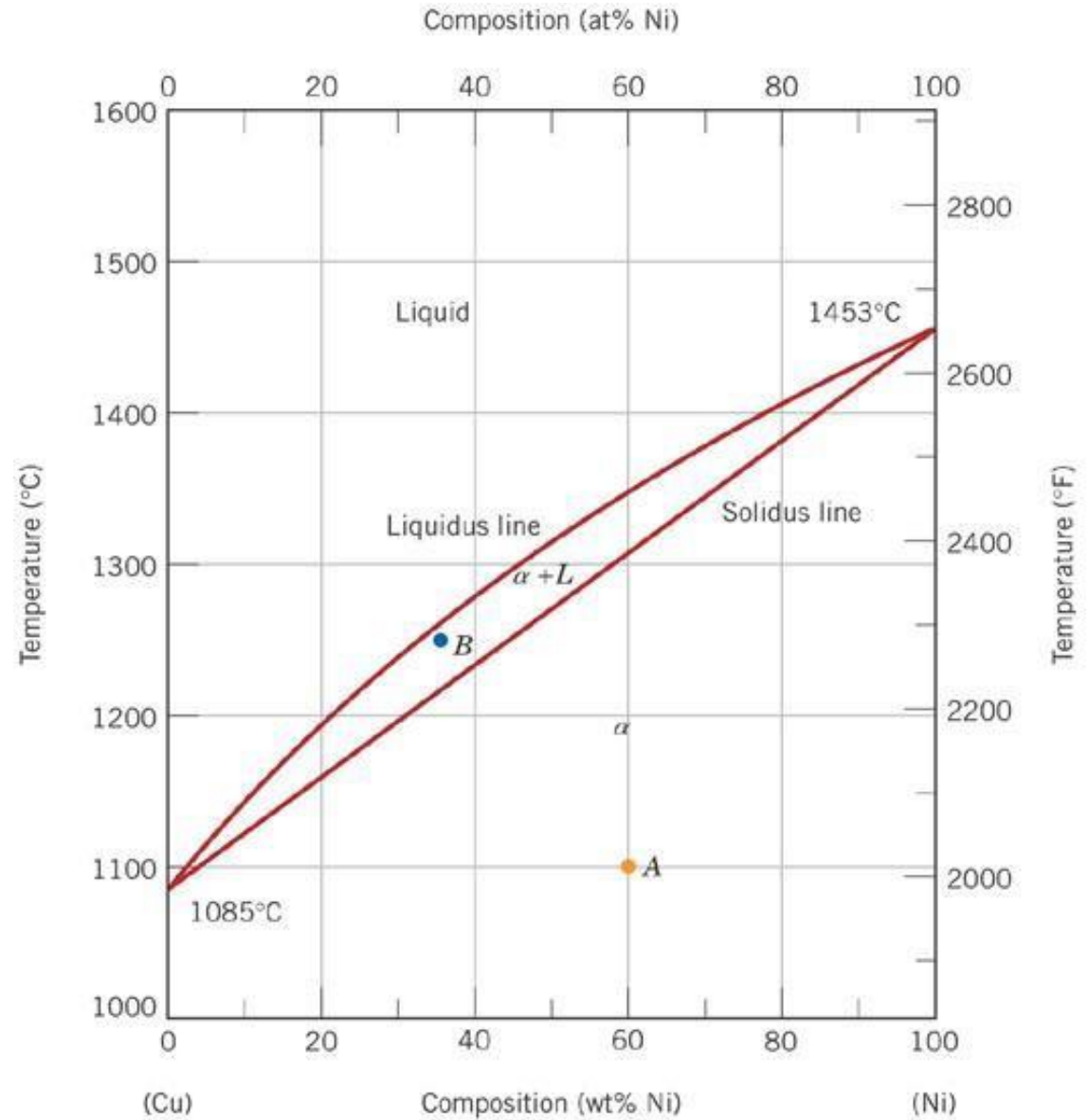
The **Hume-Rothery rules** are basic conditions for an element to dissolve in a metal, forming a substitutional solid solution.

1. The atomic radius of the solute and solvent atoms must differ by no more than 15% ($\Delta r < 15\%$).
2. The solute and solvent should have similar electronegativities.
3. Same crystal structure for “pure” metals.
4. Maximum solubility occurs when the solvent and solute have the same valence. Metals with lower valence will tend to dissolve metals with higher valence.

- Same crystal structure
- Similar electronegativities
- Similar atomic radii

	Crystal Structure	electroneg	r (nm)
Ni	FCC	1.9	0.1246
Cu	FCC	1.8	0.1278

- Ni and Cu are totally soluble in one another for all proportions.



1-D Defect : DISLOCATIONS

