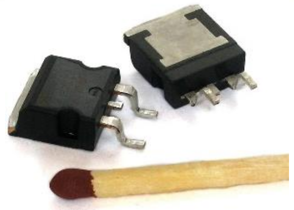
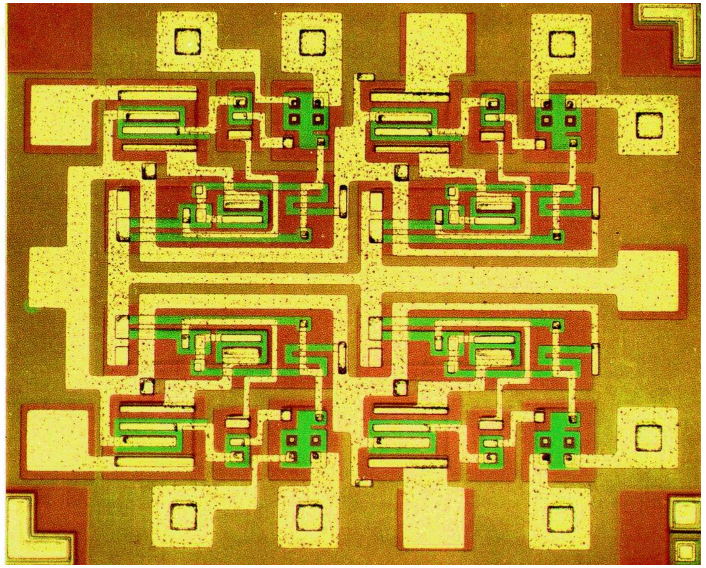
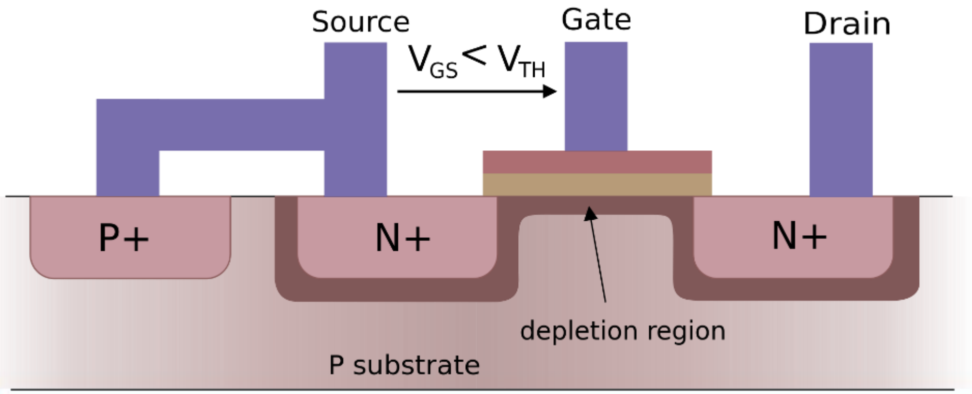
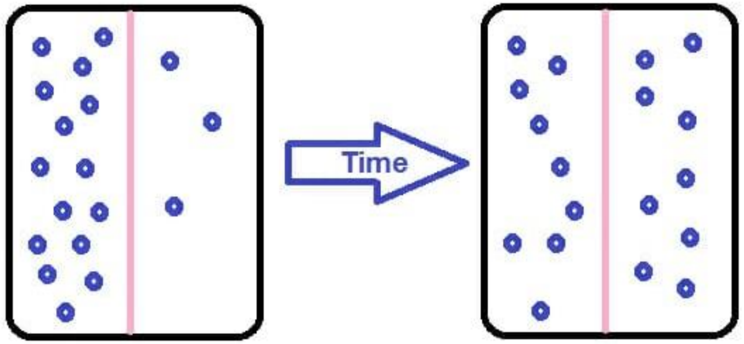


Chapter 5: Diffusion (I)



Instructor:
Prasana Kumar Sahoo
prasana@matsc.iitkgp.ac.in





What should be the properties of the Steel Gear?

Case Hardening: Hardening the surface of a metal by exposing it to impurities that diffuse into the surface region and increase surface hardness.

Common example of case hardening is carburization of steel. Diffusion of carbon atoms (interstitial mechanism) increases concentration of C atoms and makes iron (steel) harder.

Chapter Outline

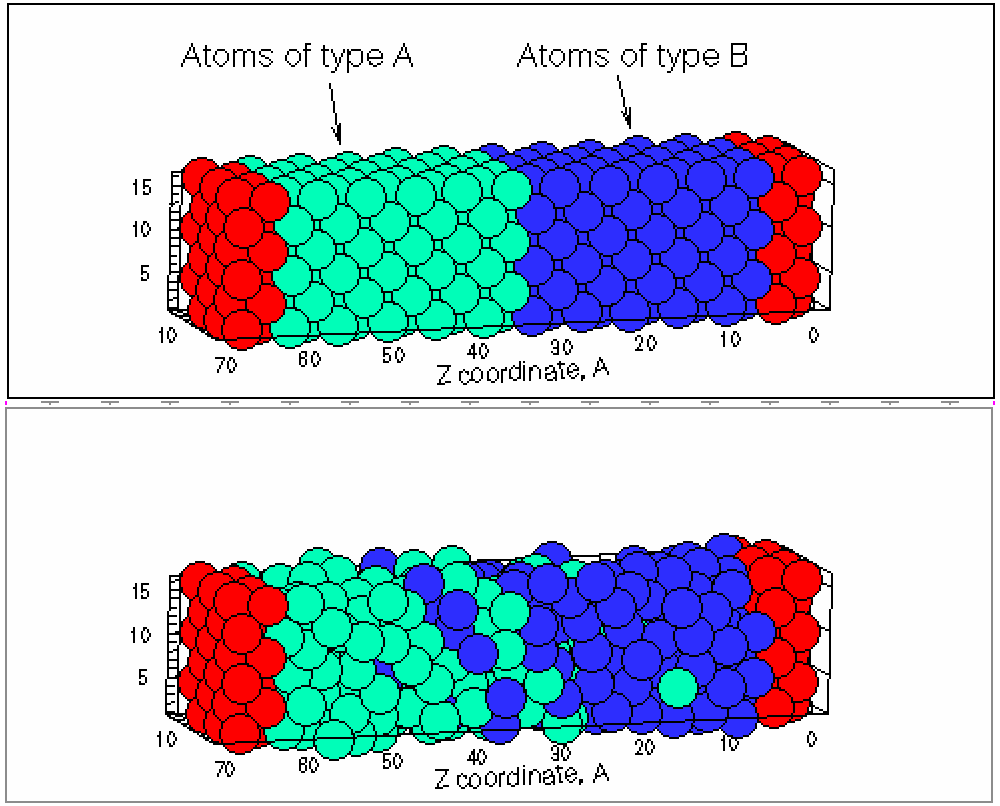
Diffusion - how do atoms move through solids?

- **Diffusion mechanisms**
  - Vacancy diffusion
  - Interstitial diffusion
  - Impurities
- **The mathematics of diffusion**
  - **Steady-state diffusion** (Fick's first law)
  - **Nonsteady-State Diffusion** (Fick's second law)
- **Factors that influence diffusion**
  - Diffusing species
  - Host solid
  - Temperature
  - Microstructure

- **Why is it an important part of processing?**
- **How can the rate of diffusion be predicted for some simple cases?**

What is diffusion?

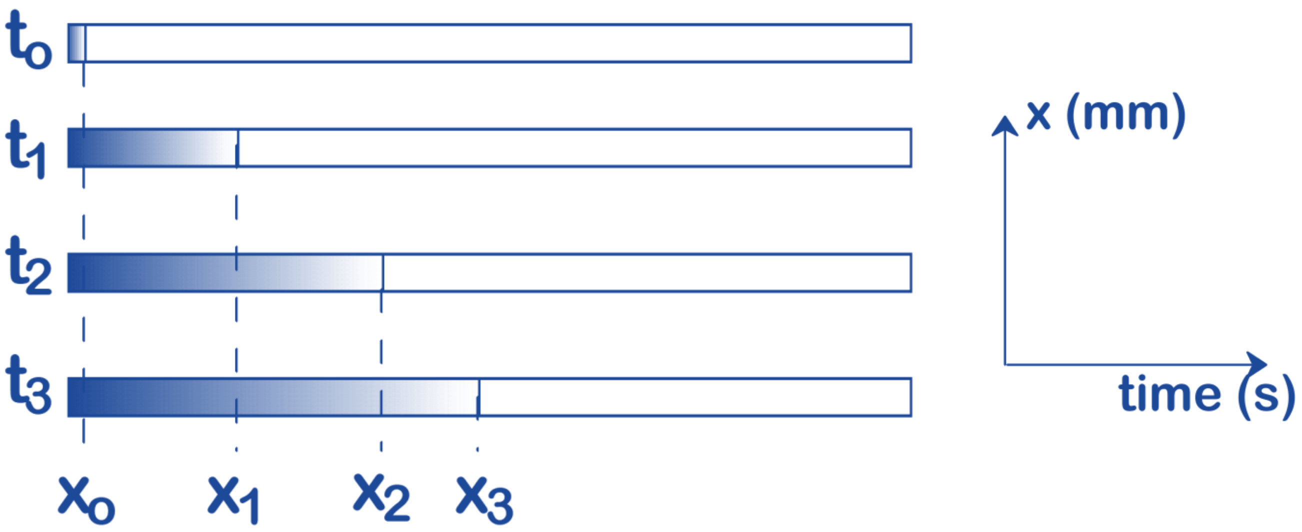
Diffusion is material transport by atomic motion.

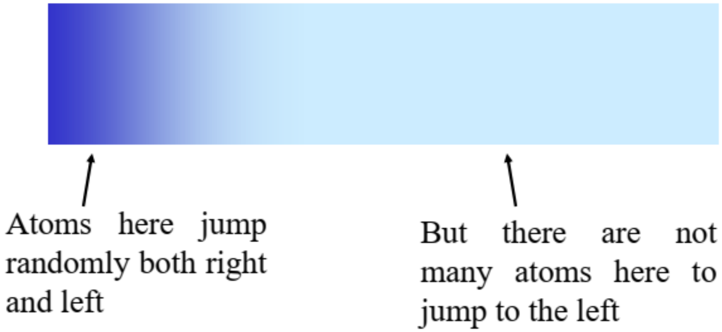


Inhomogeneous materials can become homogeneous by diffusion. For an active diffusion to occur, the temperature should be high enough to overcome energy barriers to atomic motion.

Example:

- Glass tube filled with water.
- At time t = 0, add some drops of ink to one end of the tube.
- Measure the diffusion distance, x, over some time.
- Compare the results with theory.





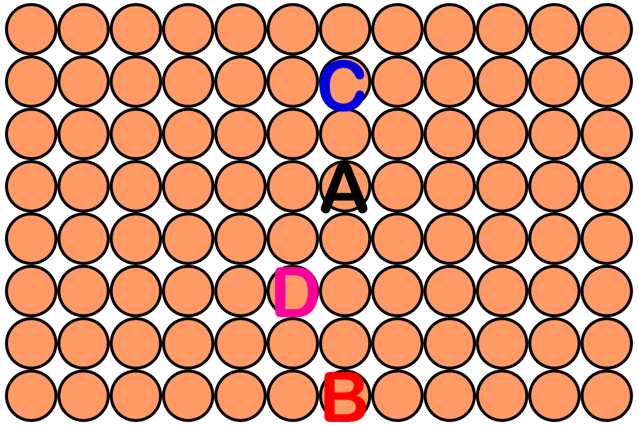
Why do the random jumps of atoms result in a flux of atoms from regions of high concentration towards the regions of low concentration?

Self-diffusion and Inter- diffusion

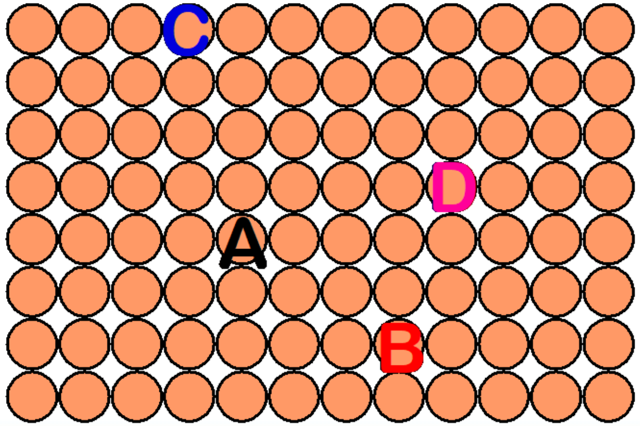
In an elemental solid, atoms also migrate.

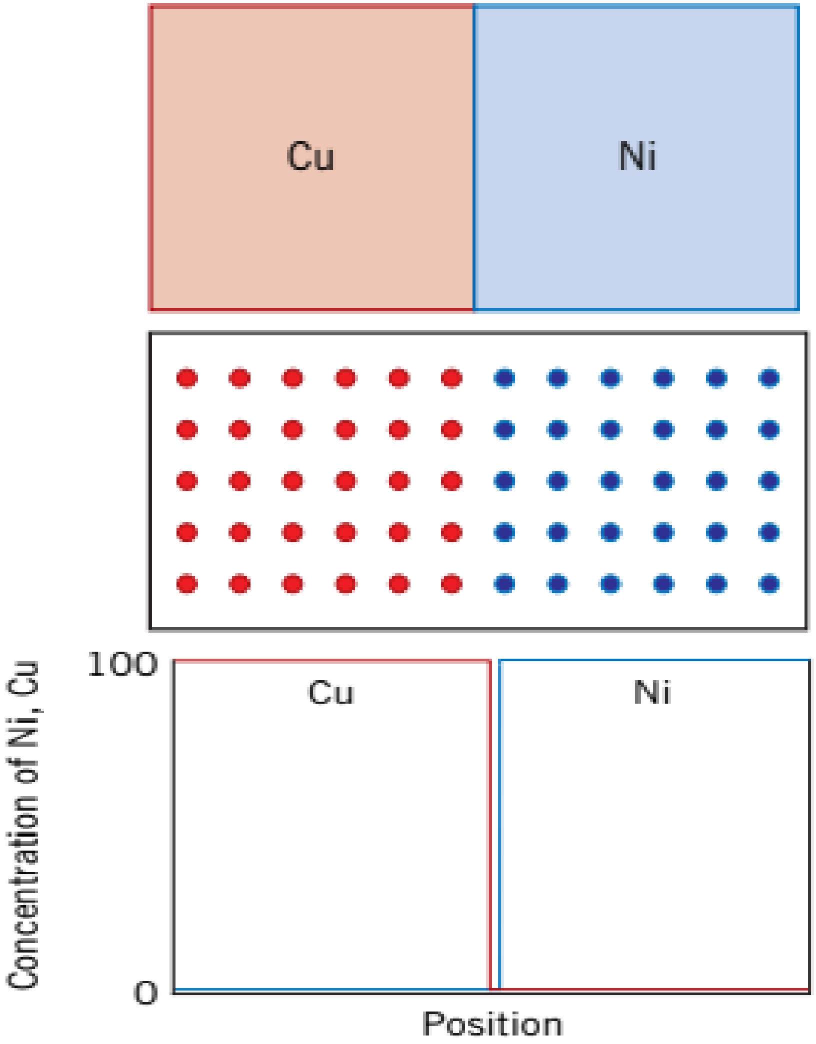
Self-diffusion is diffusion in one-component material, when all atoms that exchange positions are of the same type.

Label some atoms



After some time

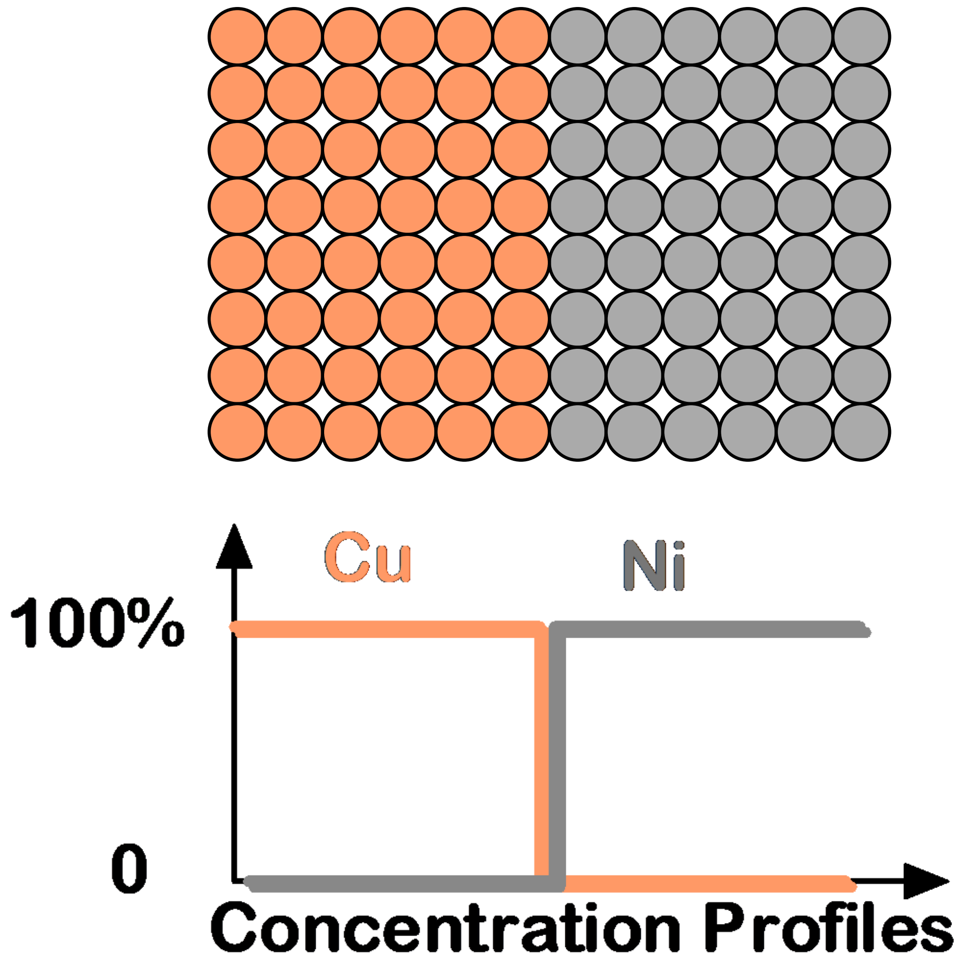




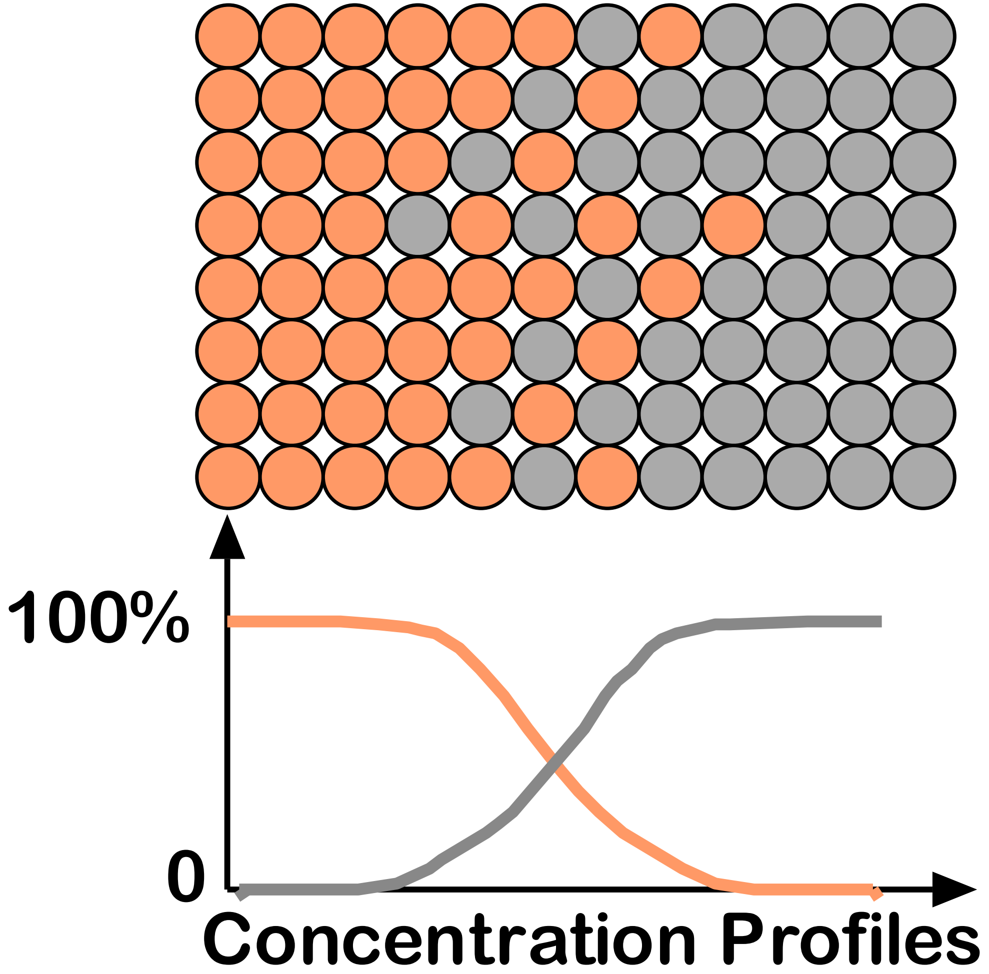
Diffusion: The Phenomena (1)

- Interdiffusion: **In an alloy, atoms tend to migrate from regions of large concentration.**

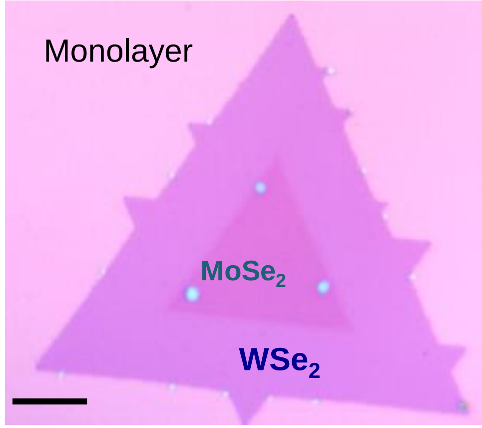
Initially



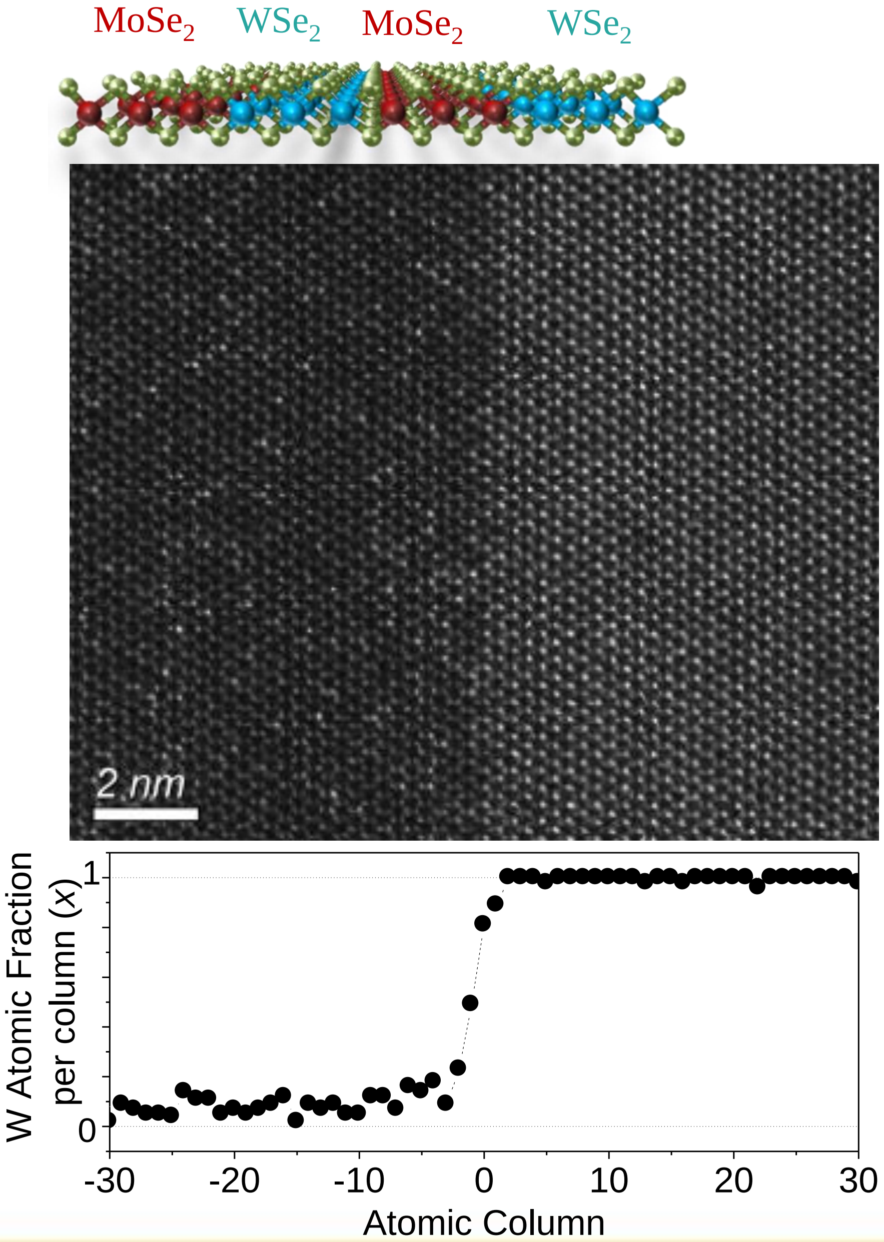
After some time

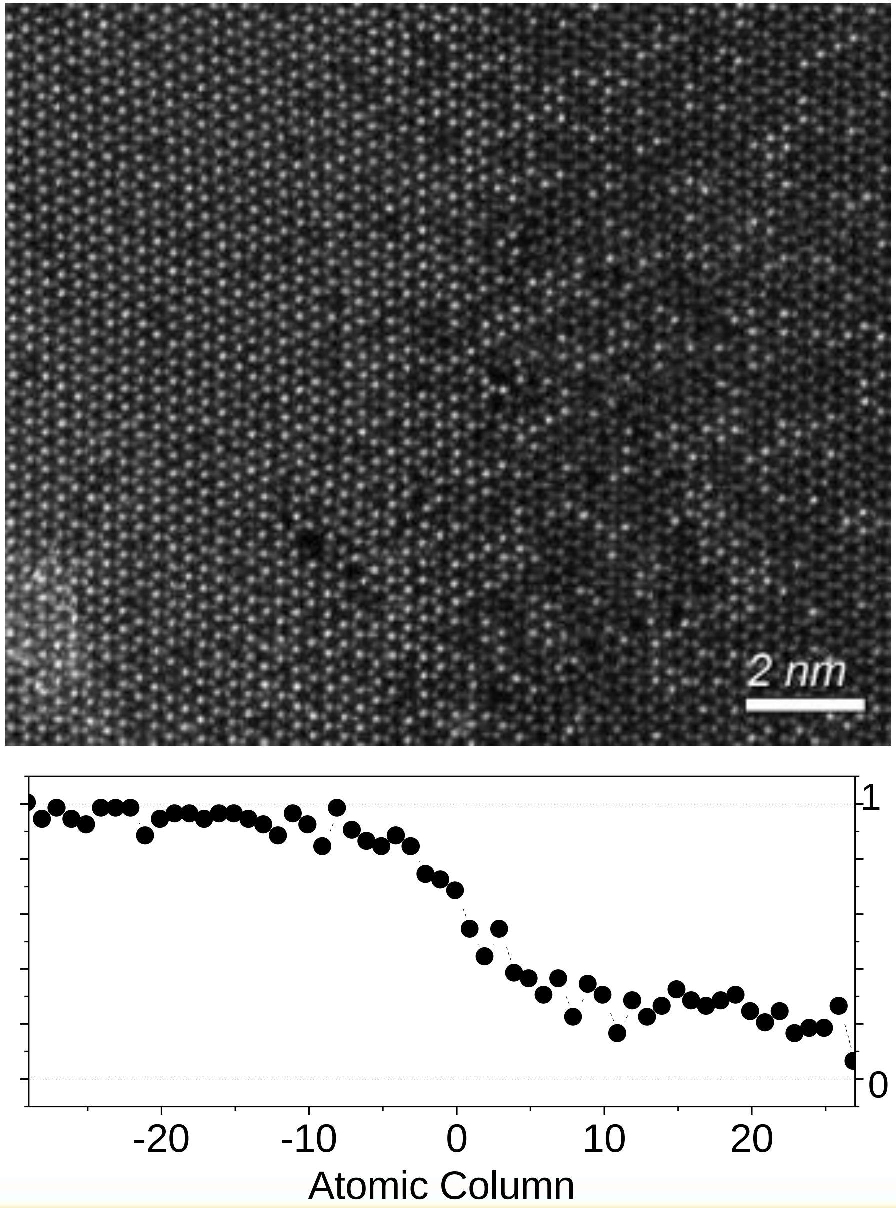


Diffusion in 2D lateral Heterostructures



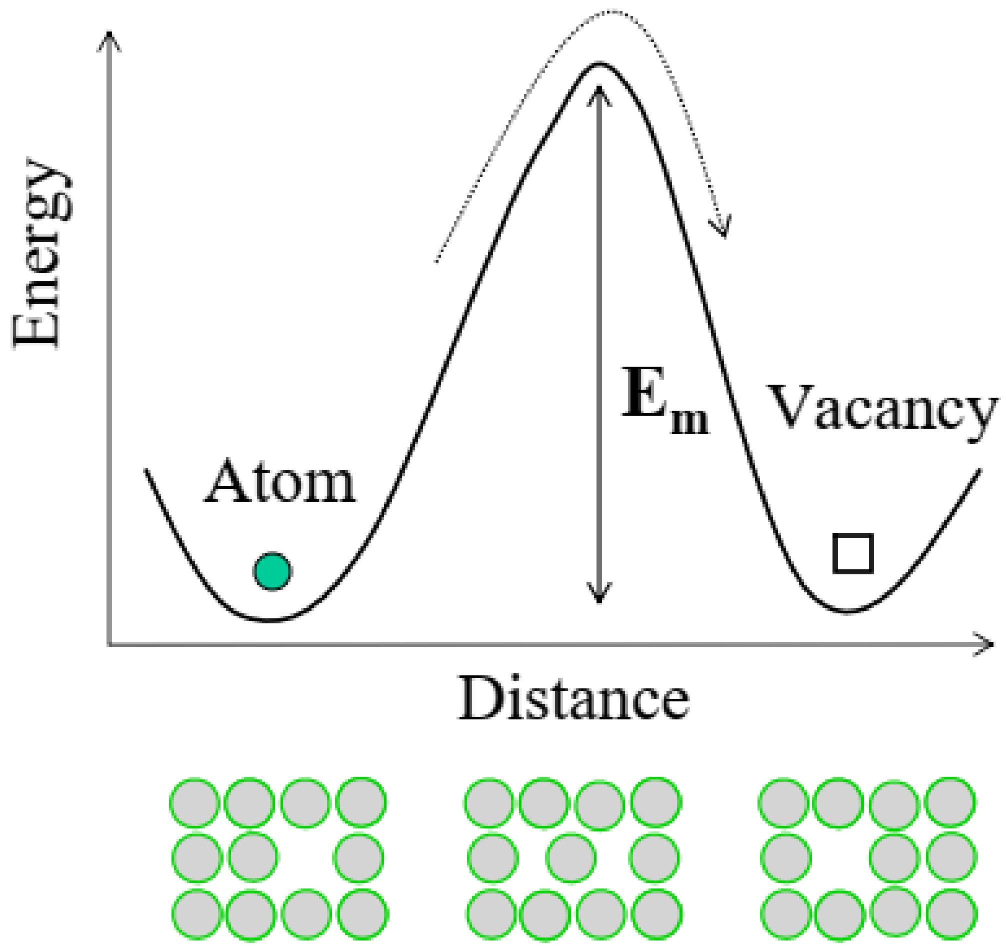
P. Sahoo *et al.*
Nature 2018





Diffusion – Thermally Activated Process

To jump from lattice site to lattice site, atoms need energy to break bonds with neighbors, and to cause the necessary lattice distortions during jump. The energy necessary for motion, Q_m, is called **the activation energy** for vacancy motion.



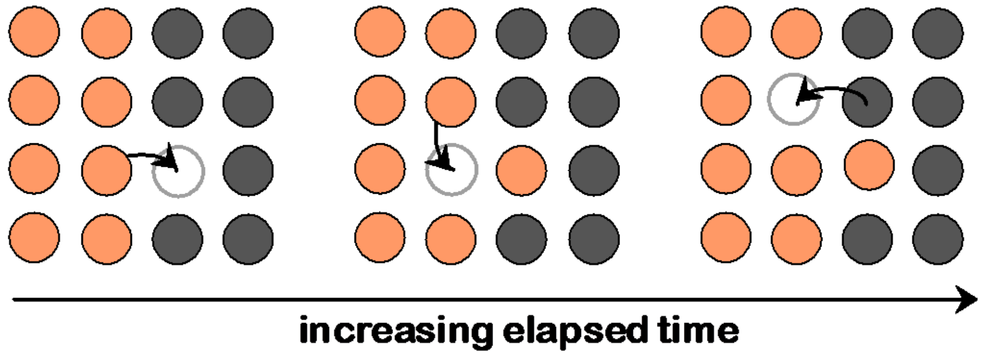
- Schematic representation of the diffusion of an atom from its original position into a vacant lattice site.

- Activation energy $\mathbf{E_m}$ has to be supplied to the atom so that it could break inter-atomic bonds and to move into the new position.

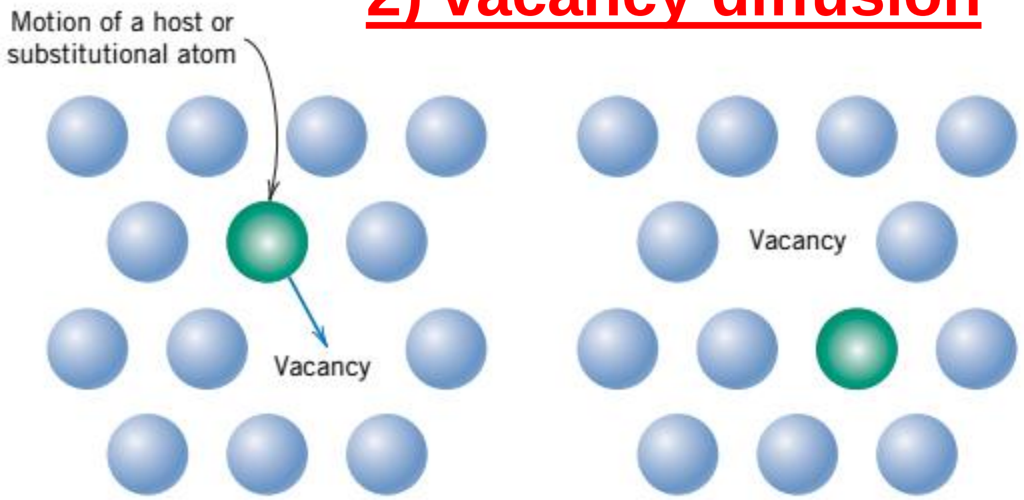
Diffusion Mechanisms

1) Substitutional Diffusion:

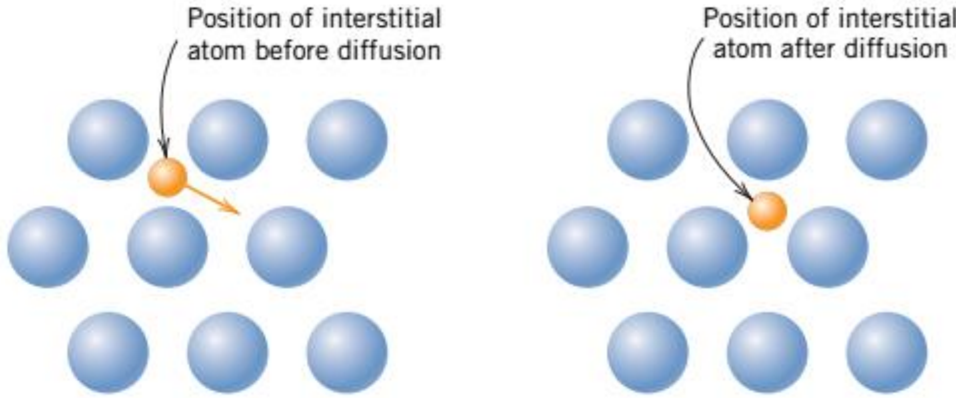
- applies to substitutional impurities
- atoms exchange with vacancies
- rate depends on:
  --number of vacancies
  --activation energy to exchange.



2) vacancy diffusion



(3) interstitial diffusion



- Interstitial diffusion is generally faster than vacancy diffusion because bonding of interstitials to the surrounding atoms is normally weaker and there are many more interstitial sites than vacancy sites to jump to.
- Requires small impurity atoms (e.g. C, H, O) to fit into interstices in host.

Processing Using Diffusion

Number (or concentration*) **of Vacancies** at T

$$c_i = \frac{n_i}{N} = e^{-\frac{\Delta E}{k_B T}}$$

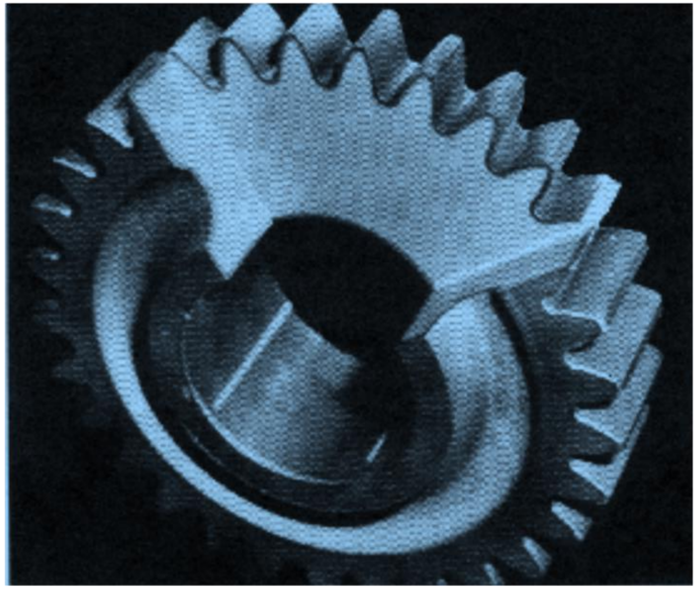
• $k_B T$ gives eV

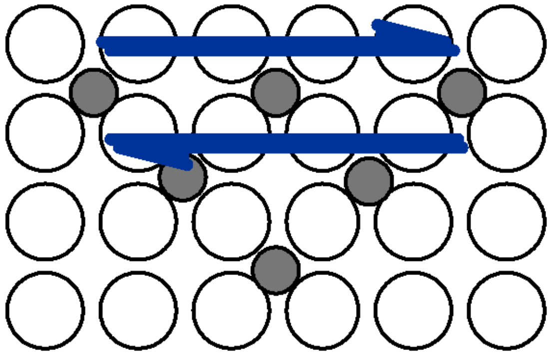
ΔE is an **activation energy** for a particular process (in J/mol, cal/mol, eV/atom).

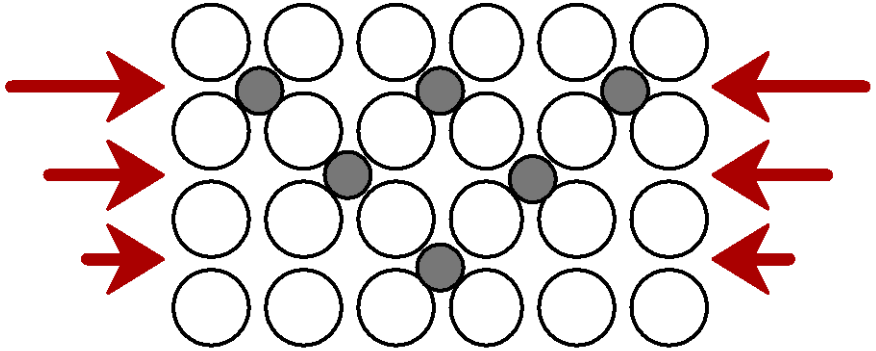
Case Hardening:

--Diffuse carbon atoms into the host iron atoms at the surface.

--Example of interstitial diffusion is a case hardened gear.





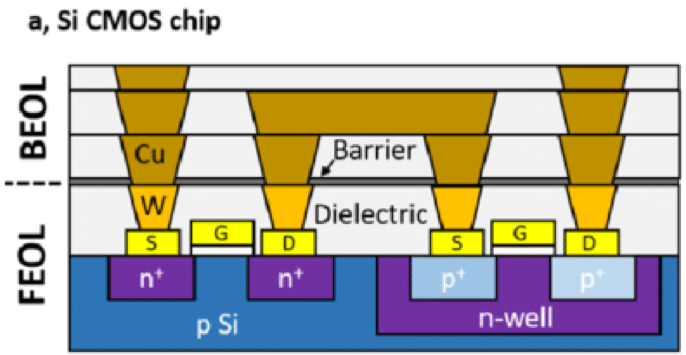


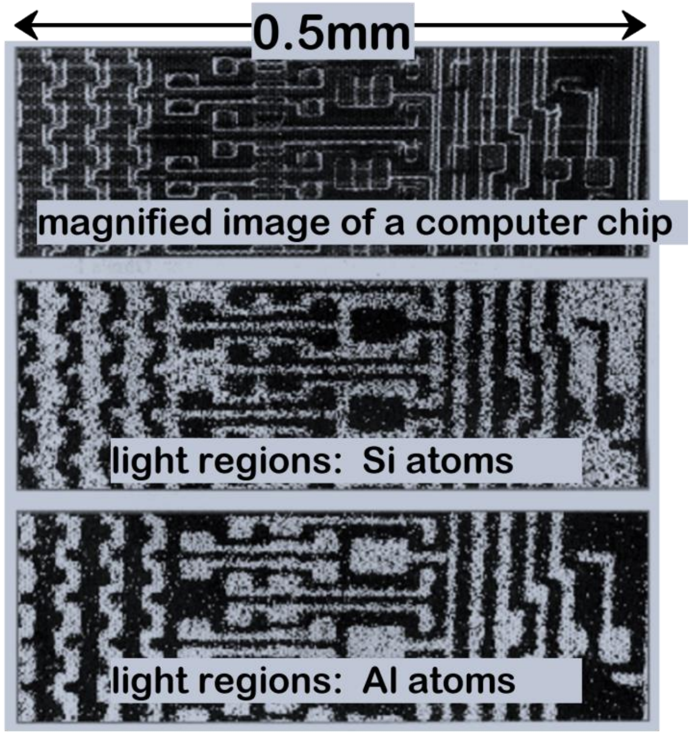
• **Result:** **The "Case" is**

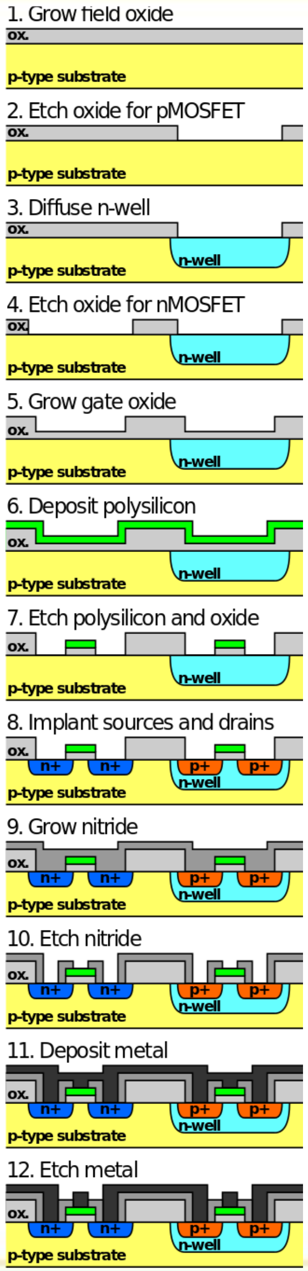
--hard to deform: C atoms "lock" planes from shearing.

--hard to crack: C atoms put the surface in compression.

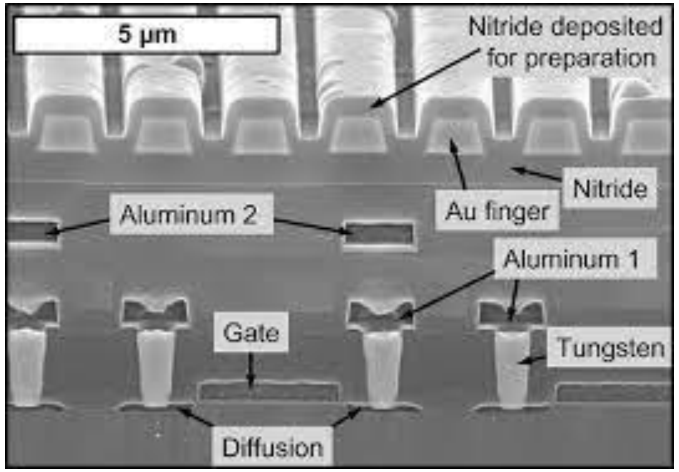
Metal–oxide–semiconductor field-effect transistor (MOSFET)

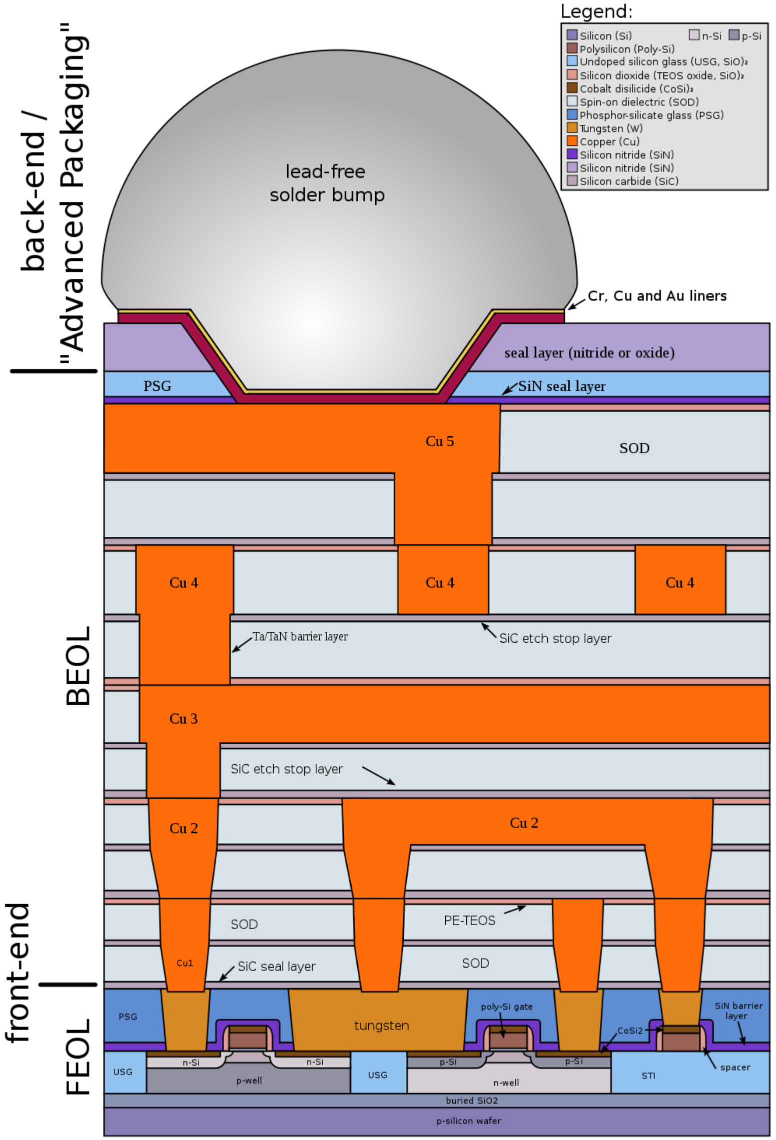






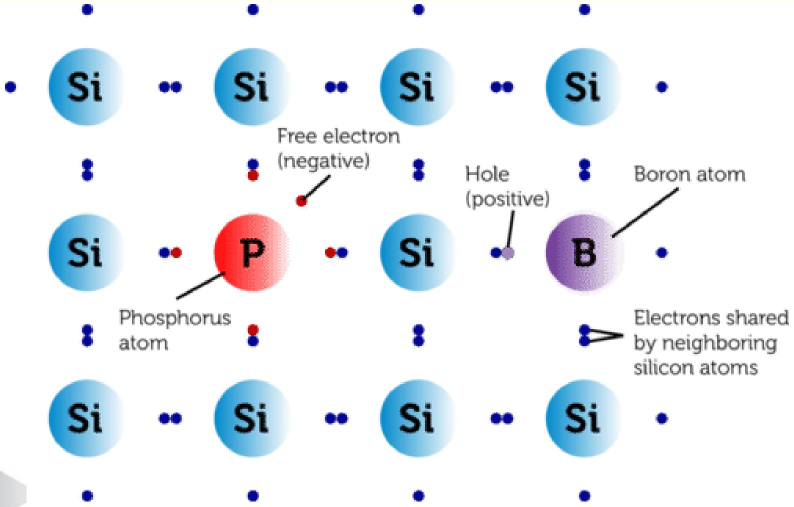
Simplified process of fabrication of a CMOS inverter on p-type substrate in semiconductor microfabrication





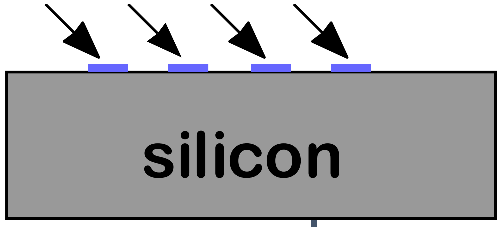
Processing Using Diffusion

Doping Silicon with P for n-type semiconductors:



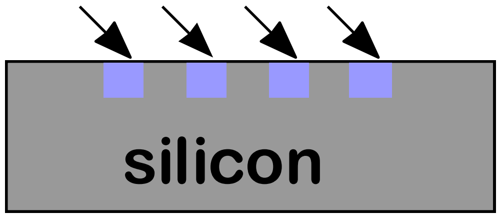
Process:

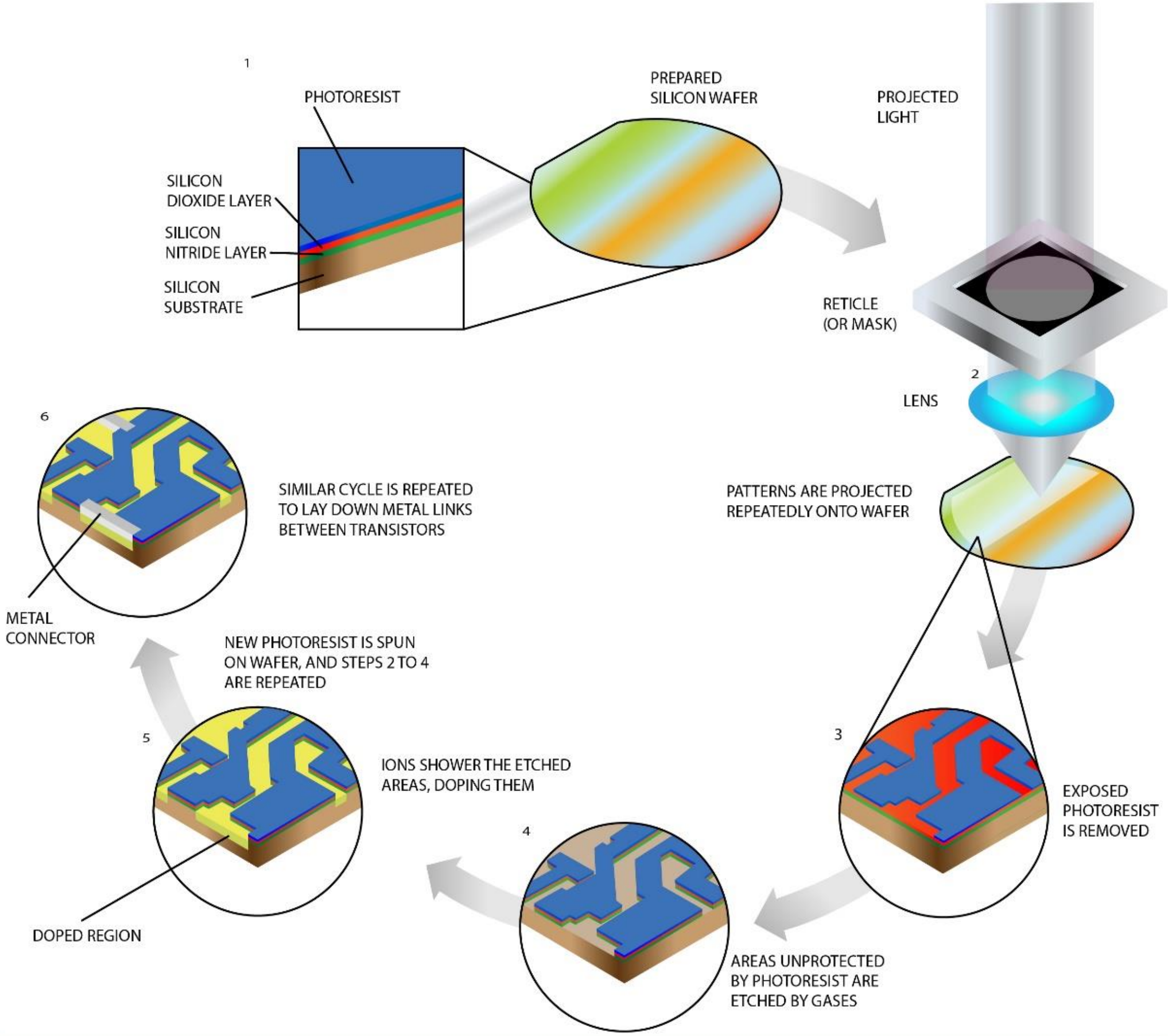
1. Deposit P rich layers on surface.



2. Heat it.

3. Result: Doped semiconductor regions.



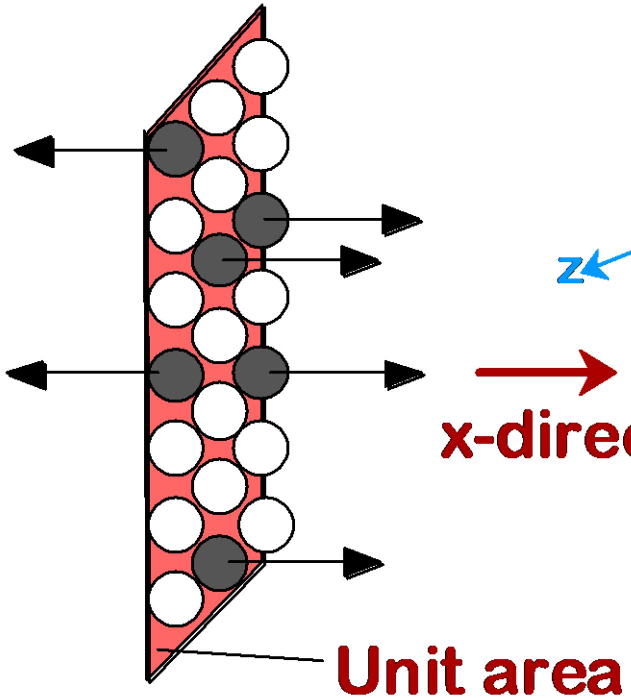


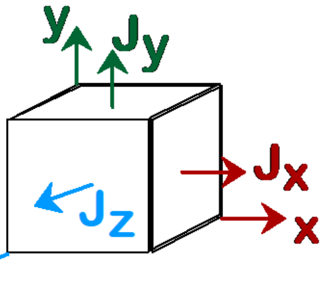
Diffusion Flux : **Fick's First Law**

Diffusion is a *time-dependent process*

Diffusion flux (J), defined as the mass (or, equivalently, the number of atoms) M diffusing through and perpendicular to a unit cross-sectional area of solid per unit of time.

$$J = \frac{1}{A}\frac{dM}{dt} \Rightarrow \left[\frac{kg}{m^2 s}\right] \text{ or } \left[\frac{atoms}{m^2 s}\right]$$





- Directional Quantity

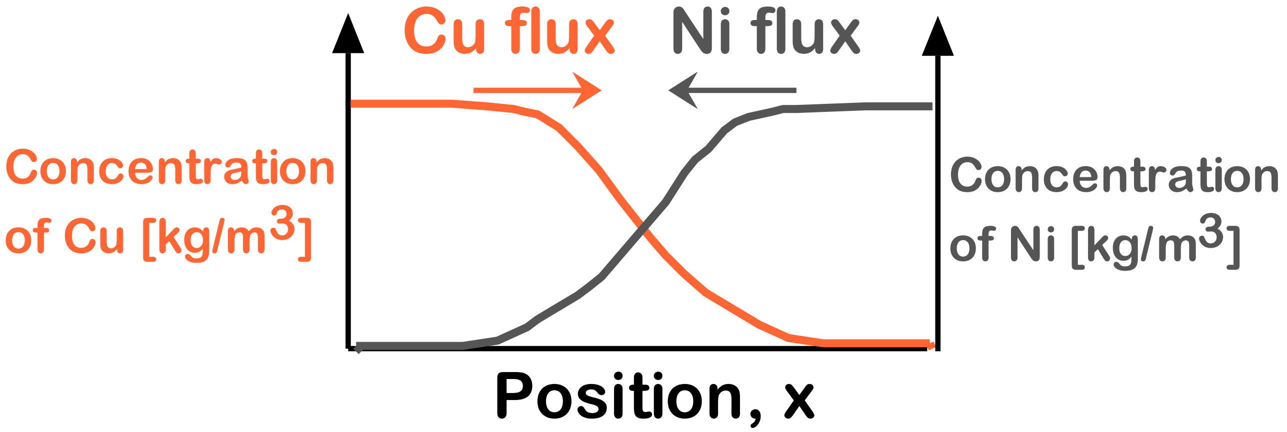
- Flux can be measured for:
  - --vacancies
  - --host (A) atoms
  - --impurity (B) atoms

- **Empirically determined**:
  - – Make thin membrane of known surface area
  - – Impose concentration gradient
  - – Measure how fast atoms or molecules diffuse through the membrane

Concentration Profiles & Flux

- **Concentration Profile, C(x): [kg/m^3]**

The mathematics of steady-state diffusion in a single (x) direction is relatively simple, in that the flux is proportional to the concentration gradient



- **Fick's First Law:**

flux in x-dir. [kg/m^2-s]

Diffusion coefficient [m^2/s]

$$J_x = -D\frac{dC}{dx}$$

concentration gradient [kg/m^4]

- **The steeper the concentration profile, the greater the flux!**
- The minus sign in the equation means that diffusion is down the concentration gradient.