EMA5001 Lecture 1
Diffusion - Introduction

Prof. Zhe Cheng

Mechanical & Materials Engineering

Florida International University

Introduction – Diffusion

❑Movement of atoms in solid materials

- Coordinated (or mechanical) movement
  - Twinning, Slipping, Martensite transformation
- Thermal movement
  - "Random walk" for each atom

❑Definition

- "…one of several transport phenomena that occur in nature. A distinguishing feature of diffusion is that it results in mixing or mass transport, without requiring bulk motion" (as opposed to convection, from Wikipedia)

❑Species that may be involved in diffusion

- Atoms
- Ions (cations, anions)
- Vacancies
- Electrons, hole
- Molecules
- …

Categories of Diffusion

- **By the uniformity of concentration**
  - Inter-diffusion: with concentration gradient
  - Self-diffusion: no concentration gradient
- **By the direction of diffusion with respect to concentration**
  - "Down-hill": from high concentration to low concentration
  - "Up-hill": from low concentration to high concentration
- **By the route of diffusion**
  - In the bulk
  - Along the surface
  - Along defects in bulk
    - Interfaces (grain boundaries)
    - Dislocations

Description & Applications of Diffusion

❑ Description of diffusion

- By a phenomenological approach
  - Fick's 1st law and 2nd law
- By physical and atomistic approach
  - Thermal random walk model

❑ Applications (list why you may be interested in diffusion)

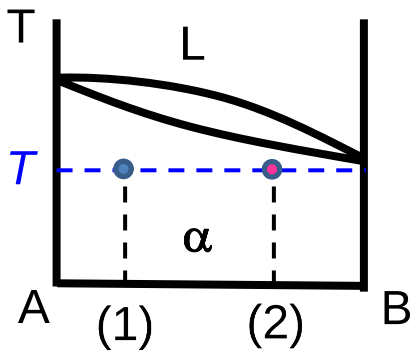
- Emitter formation in silicon solar cell
- Cu_2ZnSnS_4 absorber for thin film solar cell
- Degradation of solid oxide fuel cells
- Sintering of ultra-high temperature ceramics
- …

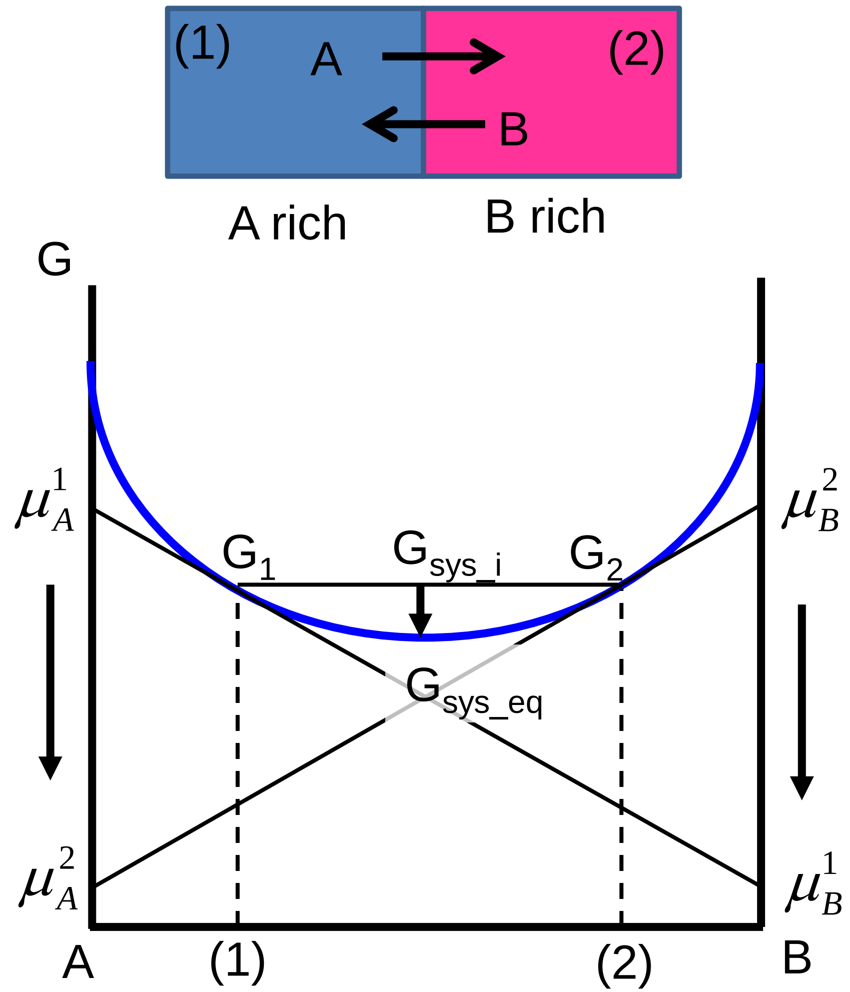
❑ Characteristics of diffusion

- Slow (relatively speaking)
- Thermally activated
- Random at individual atom (or ion, etc) level

“Down-Hill” Diffusion

❑Example #1





❑Direction

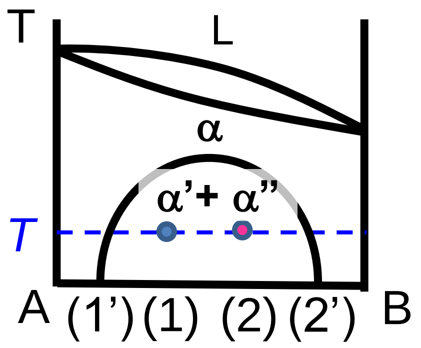
- For A: From (1) to (2)
  $X_A^1 > X_A^2 \quad \mu_A^1 > \mu_A^2$
- For B: From (2) to (1)
  $X_B^2 > X_B^1 \quad \mu_B^2 > \mu_B^1$

❑Driving force

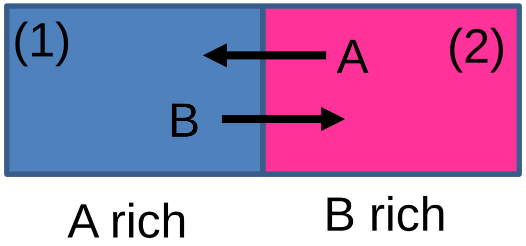
- System level: G
- Component level: μ_i

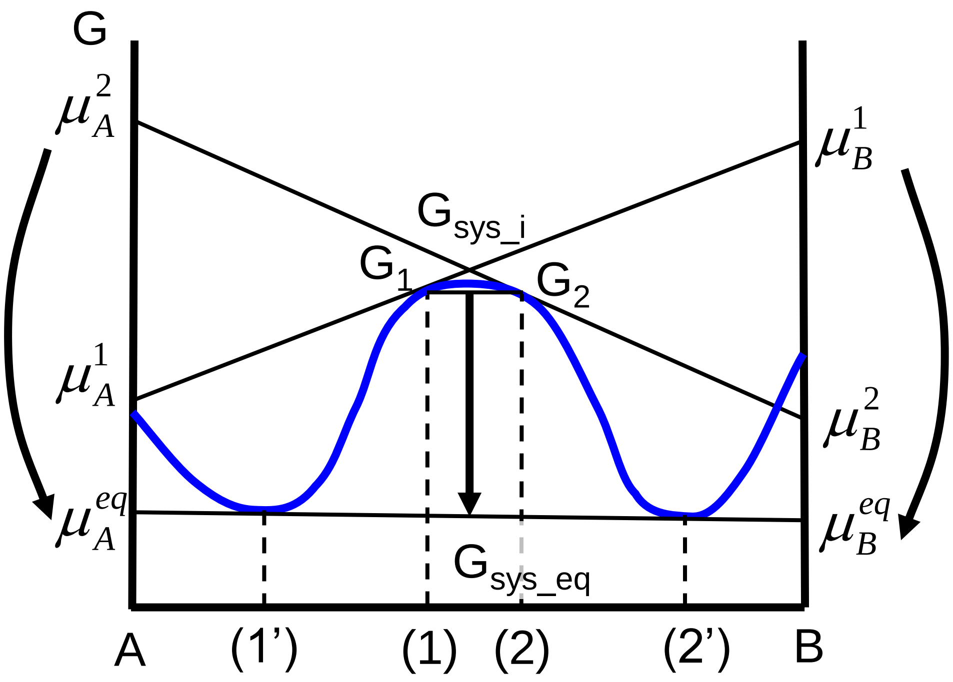
"Up-hill" Diffusion

- **Example #2**



- **Direction**
  - For A: From (2) to (1)
    $X_A^2 < X_A^1 \quad \mu_A^2 > \mu_A^1$
  - For B: From (1) to (2)
    $X_B^1 < X_B^2 \quad \mu_B^1 > \mu_B^2$
- **Driving force**
  - System level: G
  - Component level: μ_i

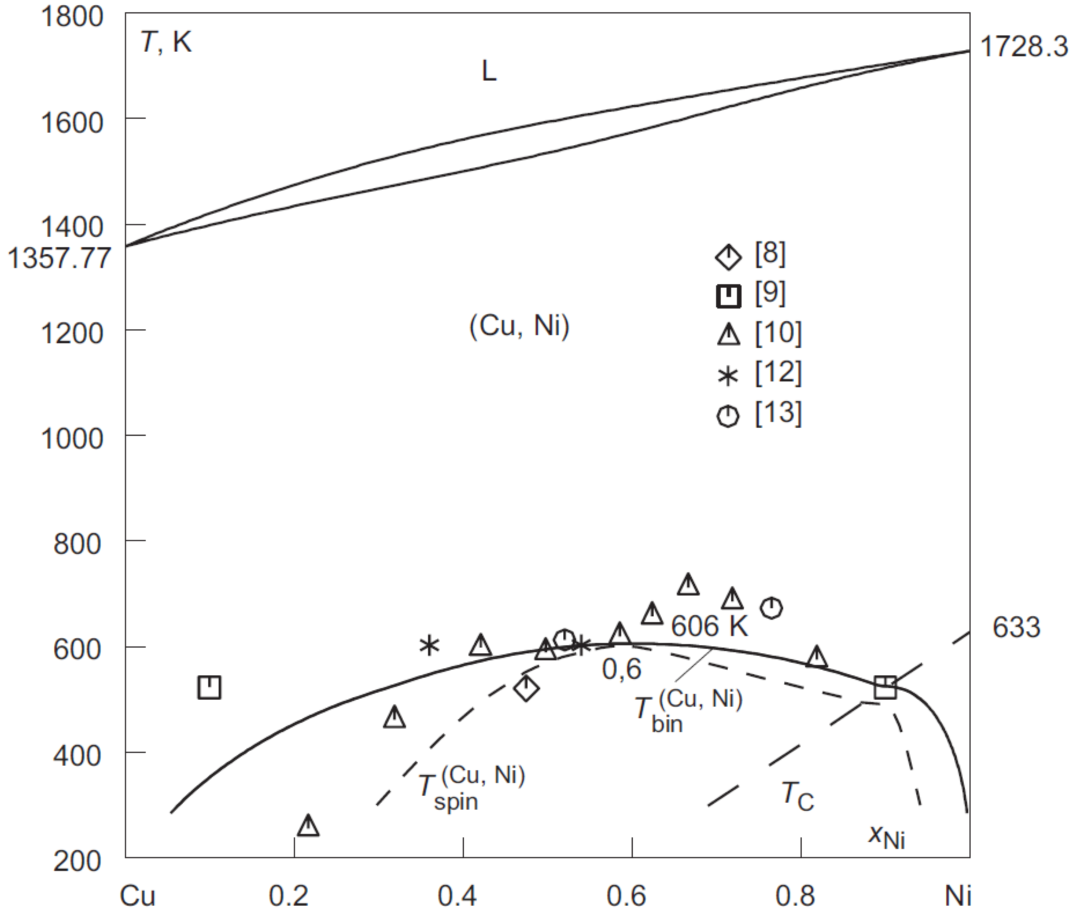




Far less common!

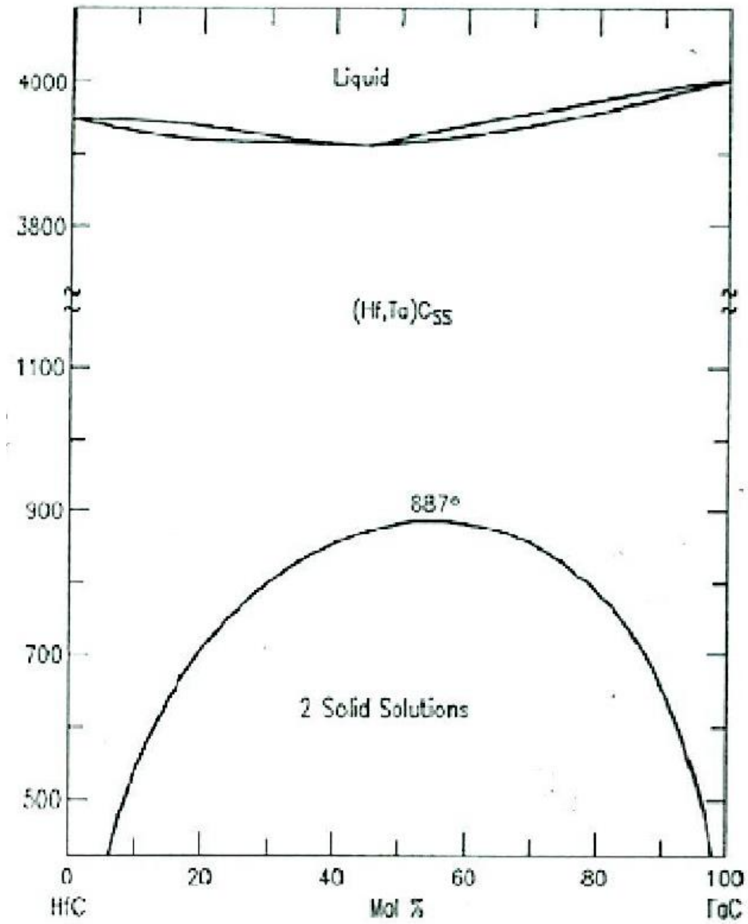
Examples

Cu-Ni



M. A. Turchanin, Powder Metallurgy and Metal Ceramics, 2007, Vol 46, Issue 9, pp 467-477

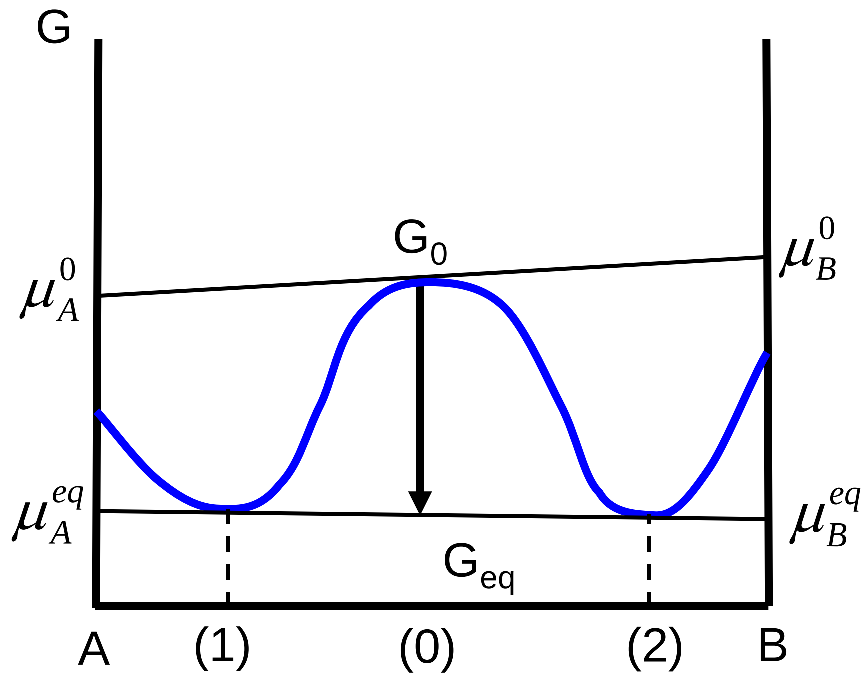
HfC-TaC



Gusev, A I .Russ. J. Phys. Chem. Vol. 59, no. 3, pp. 579. 1985

Other Considerations

- **Fundamental driving force**
  - Chemical potential
- **Diffusion ceases (theoretically):**
  - When chemical potential of components is the same everywhere
  - When system in equilibrium
- **Actual occurrence**
  - "Down-hill" - far more common
  - "Up-hill" diffusion - Rare
- **Measurement**
  - Concentration easier to measure
- **In practice**
  - Diffusion is often related to or, loosely speaking, said to be "driven by" concentration gradient



$$\mu_A^1 = \mu_A^2 = \mu_A^{eq} \qquad \mu_B^1 = \mu_B^2 = \mu_B^{eq}$$