# FYS3410 - Vår 2011 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml

Based on Introduction to Solid State Physics by Kittel

## Course content

- Periodic structures, understanding of diffraction experiment and reciprocal lattice
- Imperfections in crystals: diffusion, point defects, dislocations
- Crystal vibrations: phonon heat capacity and thermal conductivity
- Free electron Fermi gas: density of states, Fermi level, and electrical conductivity
- Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators
- Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions
- Metals: Fermi surfaces, temperature dependence of electrical conductivity

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## FYS3410 lecture schedule and exams: Spring 2011

| | | |
|---|---|---|
| W/19/1/2011: | Introduction and motivation. Periodicity and lattices | 1h |
| M/24/1/2011: | Index system for crystal planes. Crystal structures | 2h |
| W/26/1/2011: | Reciprocal space, Laue condition and Ewald construction | 1h |
| M/31/1/2011: | Brillouin Zones. Interpretation of a diffraction experiment | 2h |
| W/02/2/2011: | Crystal binding, elastic strain and waves | 1h |
| M/07/2/2011: | Elastic waves in cubic crystals; defects in crystals | 2h |
| W/09/2/2011: | Defects in crystals; case study – vacancies; diffusion | 2h |
| M/14/2/2011: | Crystal vibrations and phonons | 2h |
| W/16/2/2011: | Lattice heat capacity: Dulong-Petit and Einstein models | 2h |
| M/21/2/2011: | Phonon density of states (DOS) and Debye model | 2h |
| W/23/2/2011: | General result for DOS; role of anharmonic interactions | 2h |
| M/28/2/2011: | Thermal conductivity and repetition of crystal vibrations | 2h |
| W/02/3/2011: | no lectures | |
| M/07/3/2011: | no lectures | |
| W/09/3/2011: | no lectures | |
| M/14/3/2011: | Free electron Fermi gas in 1D and 3D – ground state | 2h |
| W/17/3/2011: | Density of states, effect of temperature – FD distribution | 1h |
| M/21/3/2011: | Heat capacity of FEFG | 2h |
| W/23/3/2011: | Repetition | 1h |
| M/28/3/2011: | Mid-term exam | |

| | | |
|---|---|---|
| M/04/4/2011: | Electrical and thermal conductivity in metals | 2h |
| W/06/4/2011: | Bragg reflection of electron waves at the boundary of BZ | 2h |
| M/11/4/2011: | Energy bands, Kronig - Penny model | 2h |
| W/13/4/2011: | Empty lattice approximation; number of orbitals in a band | 2h |
| Påsk uppehåll | | |
| W/27/4/2011 | no lectures | |
| M/02/5/2011: | no lectures | |
| W/04/5/2011: | no lectures | |
| M/09/5/2010: | Semiconductors, effective mass method, intrinsic carriers | 2h |
| W/11/4/2010: | Impurity states in semiconductors and carrier statistics | 2h |
| M/16/5/2010: | p-n junctions, Schottky contacts and heterojunctions | 2h |
| W/18/5/2010: | Metals and Fermi surfaces | 1h |
| M/23/5/2010: | Repetition | 2h |
| 26-27/5/2010: | Final Exam (sensor:???) | |

# Lecture 9: Diffusion

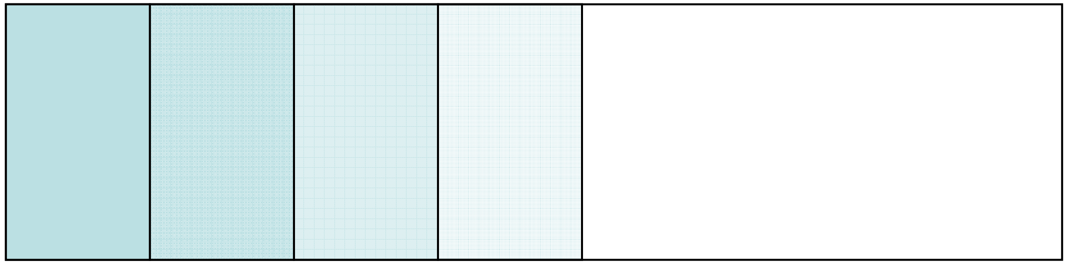
- Phenomenology of diffusion: describing diffusion in terms of diffusion flux
- Microscopic diffusion mechanisms
- Sb diffusion as a function of temperature as stress in Si/SiGe heterostructures

# Lecture 9: Diffusion

- **Phenomenology of diffusion: describing diffusion in terms of diffusion flux**
- **Microscopic diffusion mechanism**
- **Sb diffusion as a function of temperature as stress in Si/SiGe heterostructures**

# Diffusion

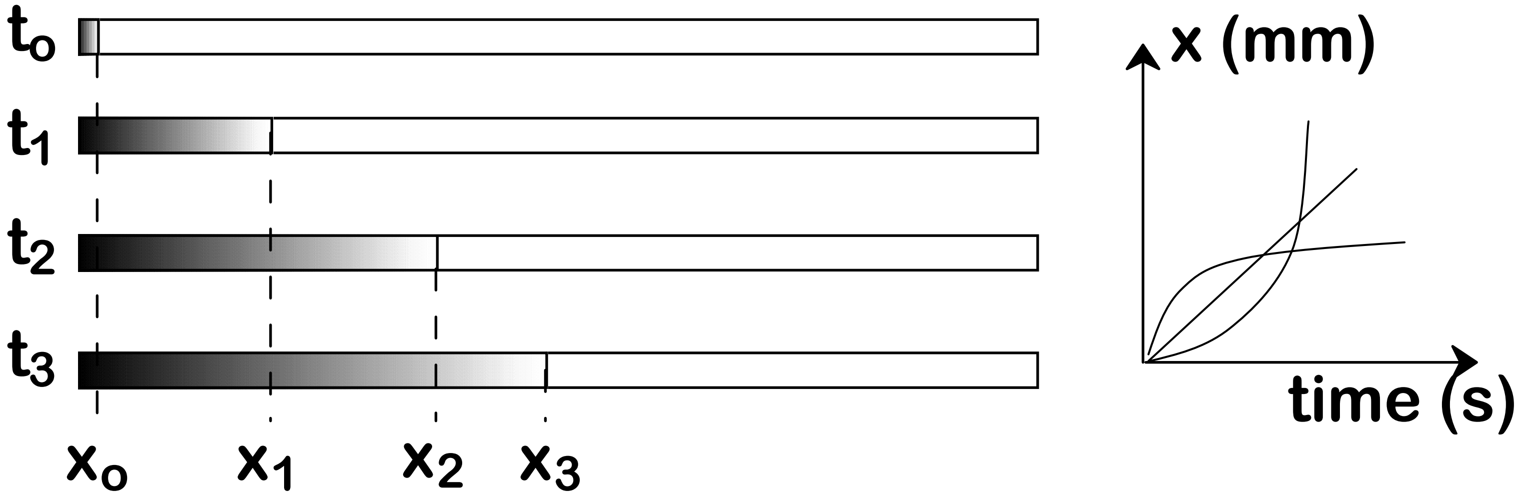
Phenomenon of material transport by atomic or particle transport from region of high to low concentration



- What forces the particles to go from left to right?
- Does each particle “know” its local concentration?
- Every particle is equally likely to go left or right!
- At the interfaces in the above picture, there are **more** particles going right than left ➔ this causes an average “flux” of particles to the right!
- Largely determined by probability & statistics

# Diffusion

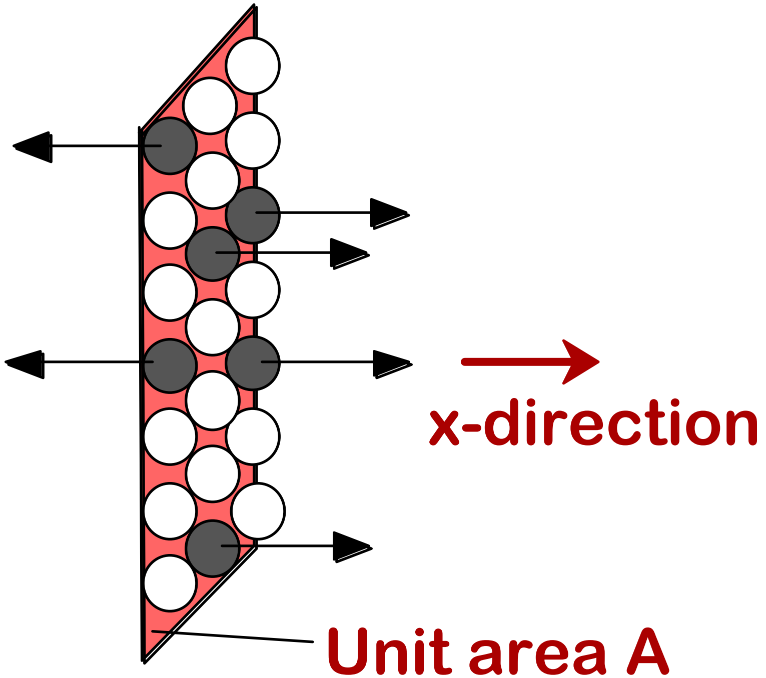
- Glass tube filled with water.
- At time $t = 0$, add some drops of ink to one end of the tube.
- Measure the diffusion distance, $x$, over some time.



# Describing diffusion in terms of diffusion flux

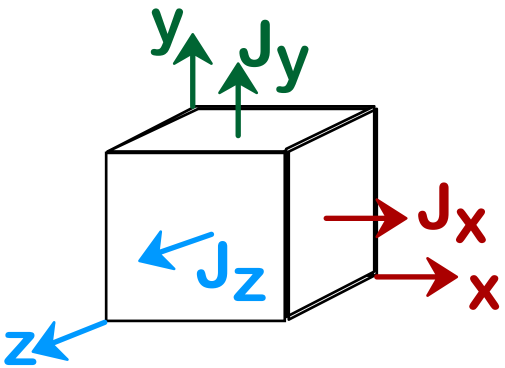
- Flux: amount of material or atoms moving past a unit area in unit time
  Flux, J = ΔM/(A Δt)

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



Unit area A through which atoms move.

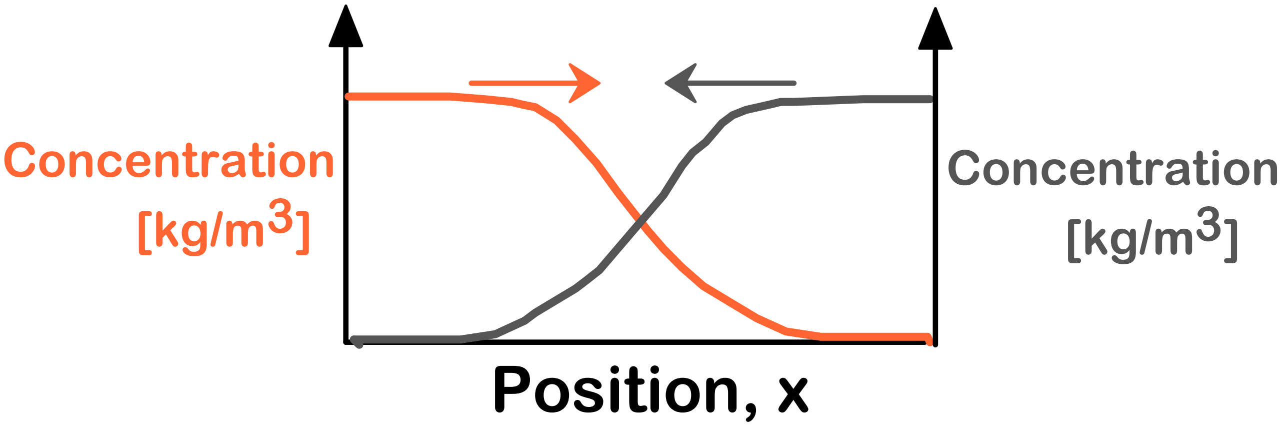
- Directional Quantity



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

# Describing diffusion in terms of diffusion flux

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



- Fick's First Law:

flux in x-dir. [kg/m$^2$-s] → $J_x$

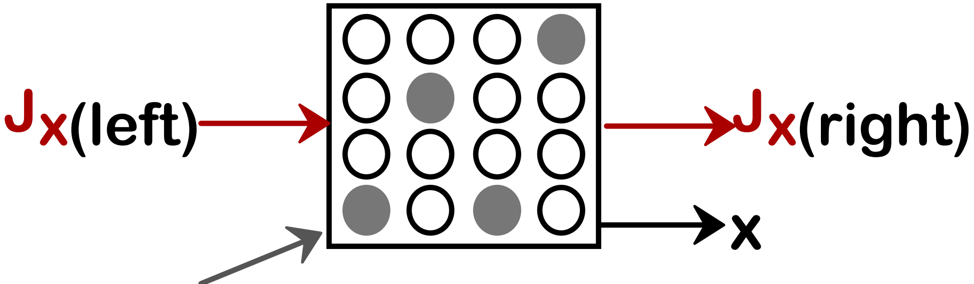
Diffusion coefficient [m$^2$/s] → D

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

concentration gradient [kg/m$^4$] → $\frac{dC}{dx}$

# Describing diffusion in terms of diffusion flux

- Steady State: Steady rate of diffusion from one end to the other. Implies that the concentration profile doesn't change with time. Why?



**$J_x$(left)** **$J_x$(right)** **x**

**Steady State:**

**$J_x$(left) = $J_x$(right)**

**Concentration, C, in the box doesn't change w/time.**

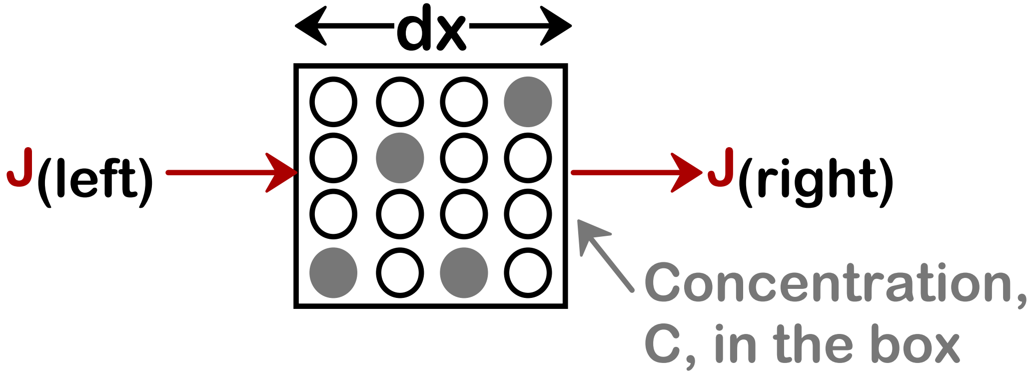
- Apply Fick's First Law: $J_x = -D\frac{dC}{dx}$

- If $J_x)_{left} = J_x)_{right}$ , then $\left(\frac{dC}{dx}\right)_{left} = \left(\frac{dC}{dx}\right)_{right}$

- Result: the slope, dC/dx, must be constant (i.e., slope doesn't vary with position)!

# Describing diffusion in terms of diffusion flux

- Concentration profile, C(x), changes w/ time.



- To conserve matter:

$$\boxed{\frac{J(\text{right}) - J(\text{left})}{dx}} = -\frac{dC}{dt}$$

$$\boxed{\frac{dJ}{dx}} = -\frac{dC}{dt}$$

- Fick's First Law:

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

$$\boxed{\frac{dJ}{dx}} = -D\frac{d^2C}{dx^2}$$

(if D does not vary with x)

equate

- Governing Eqn.:

$$\boxed{\frac{dC}{dt} = D\frac{d^2C}{dx^2}}$$

Fick’s second law

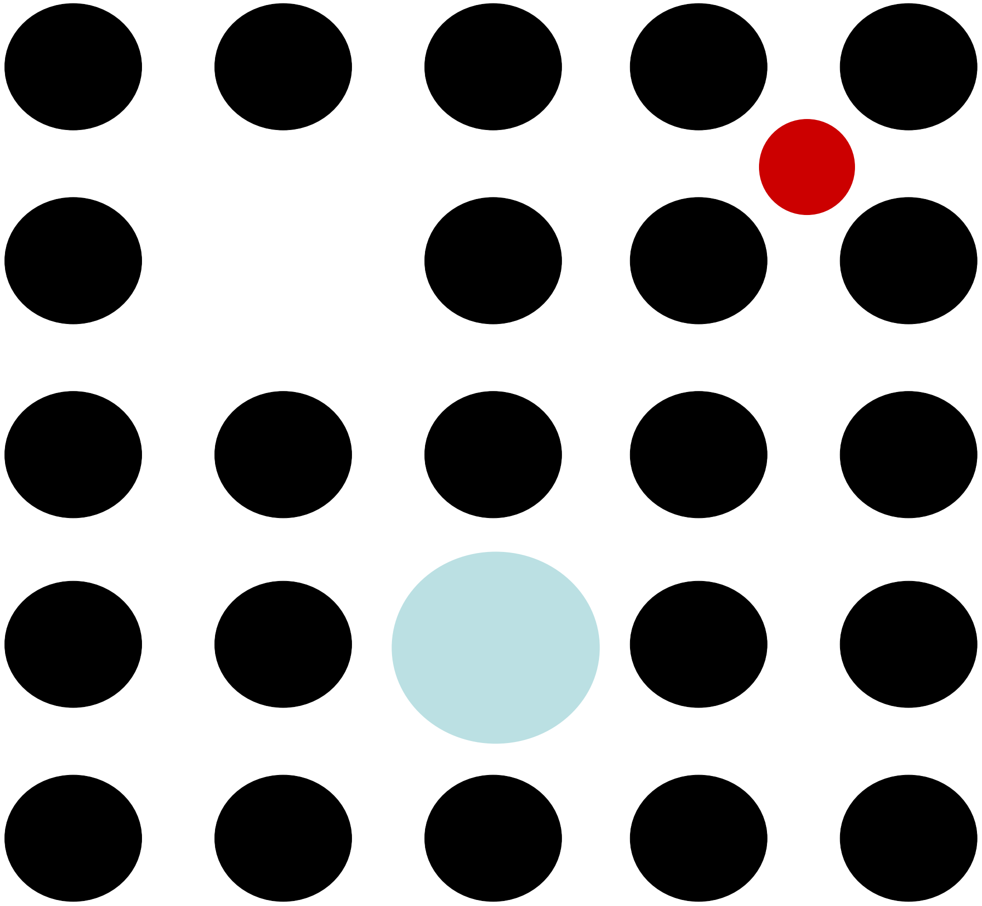
# Lecture 9: Diffusion

- Phenomenology of diffusion: describing diffusion in terms of diffusion flux

- **Microscopic diffusion mechanisms**

- Sb diffusion as a function of temperature as stress in Si/SiGe heterostructures

# Type of point defects



**vacancy**

**Interstitial impurity**

**Substitutional impurity**

# Diffusion mechanisms

Diffusion at the atomic level is a step-wise migration of atoms from lattice site to lattice site

Conditions for diffusion:

- there must be an adjacent empty site
- atom must have sufficient energy to break bonds with its neighbors and migrate to adjacent site (“activation” energy)

Higher the temperature, higher is the probability that an atom will have sufficient energy

➔ hence, diffusion rates increase with temperature

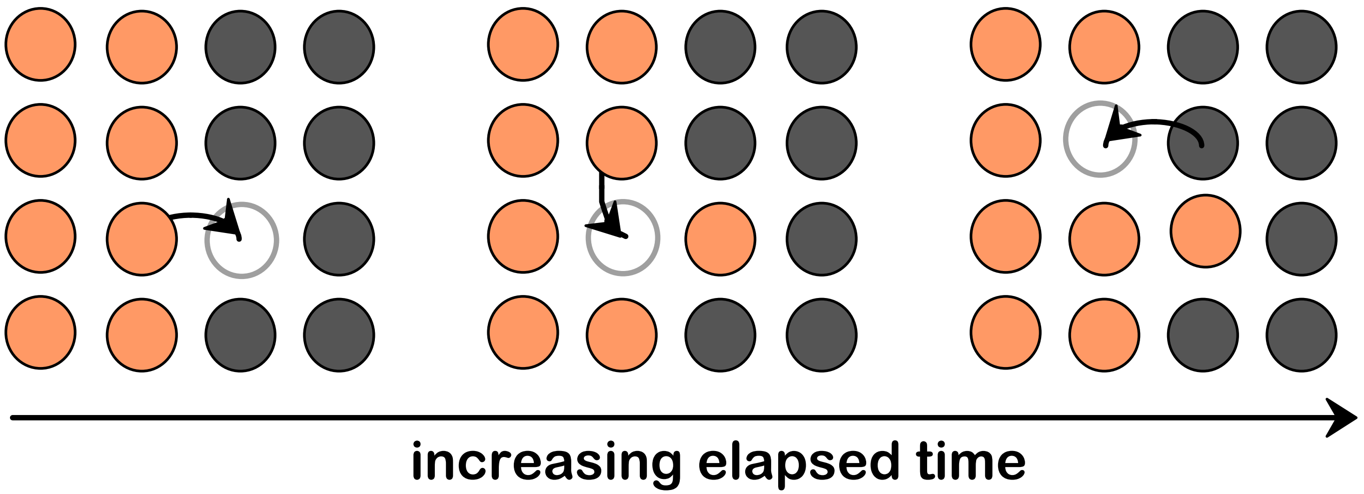
Types of atomic diffusion mechanisms:

- substitutional (through vacancies)
- interstitial

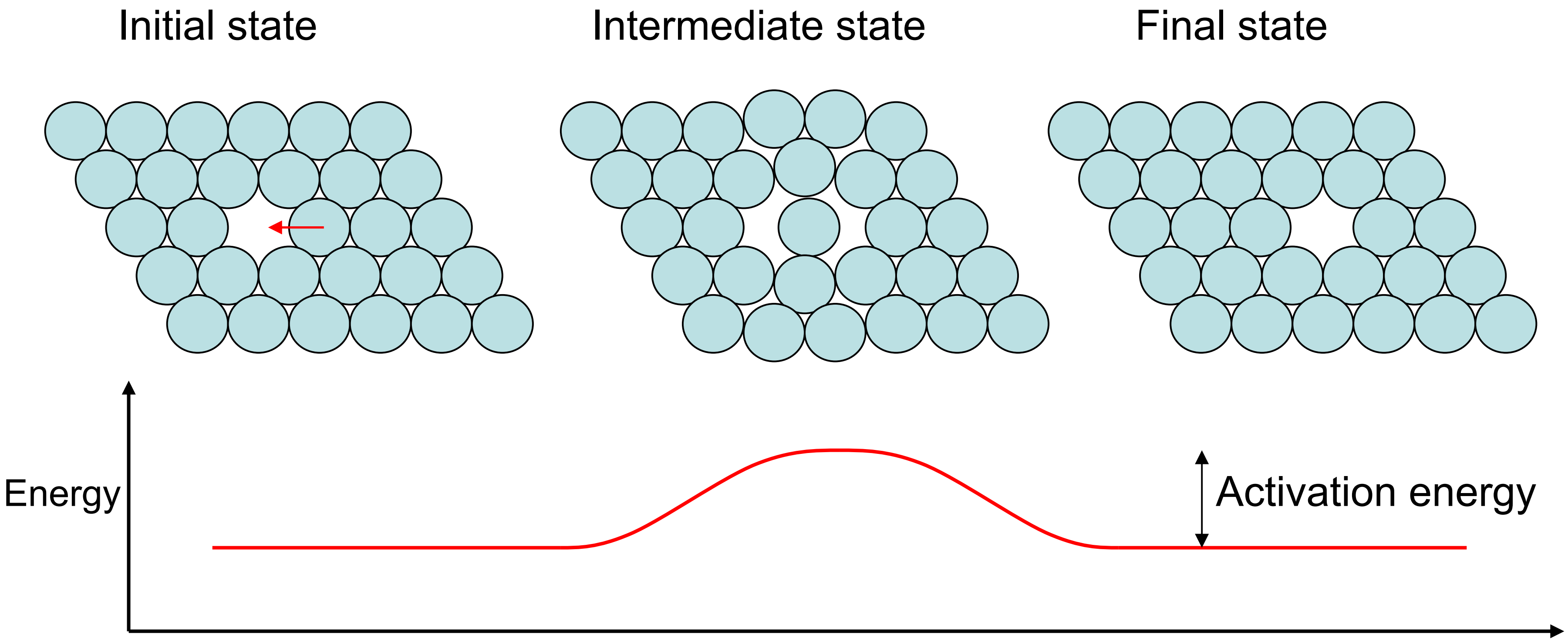
# Diffusion mechanisms

## Substitutional Diffusion:

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


increasing elapsed time

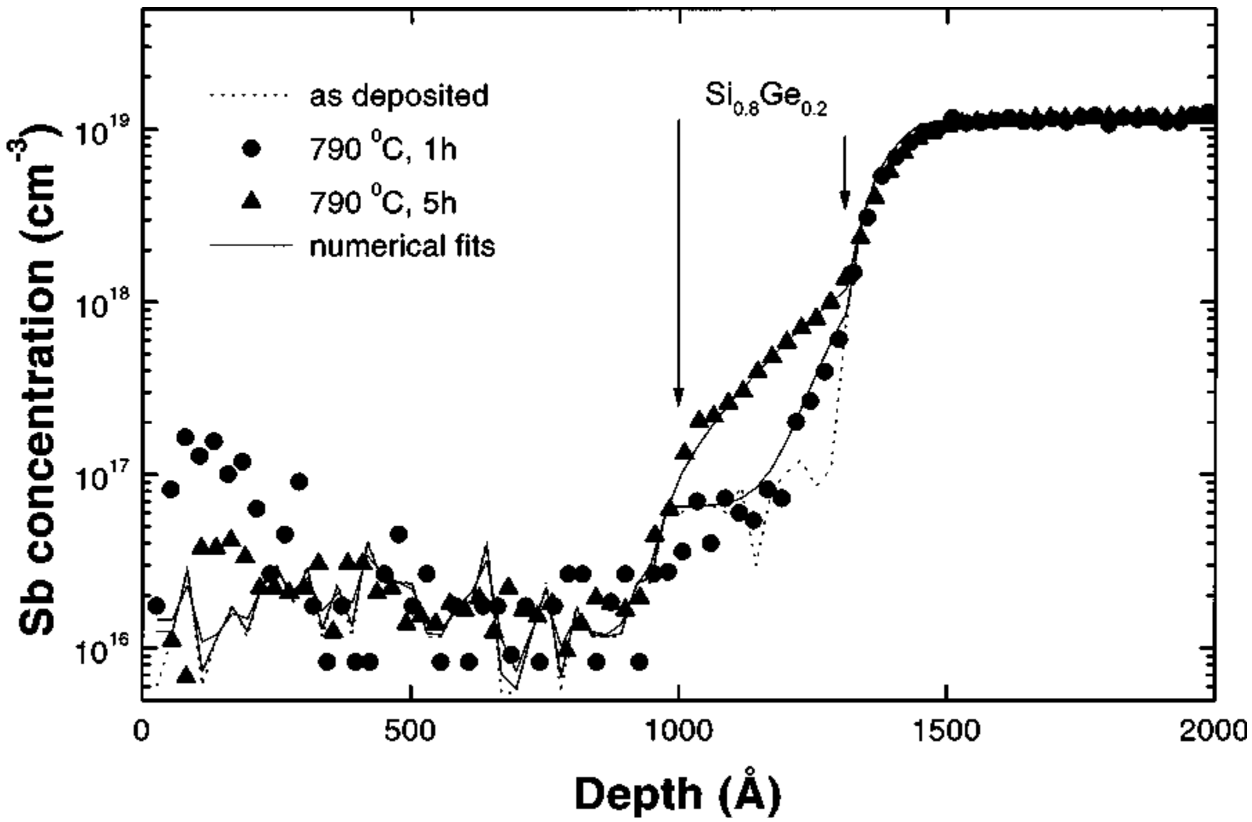
# Diffusion mechanisms

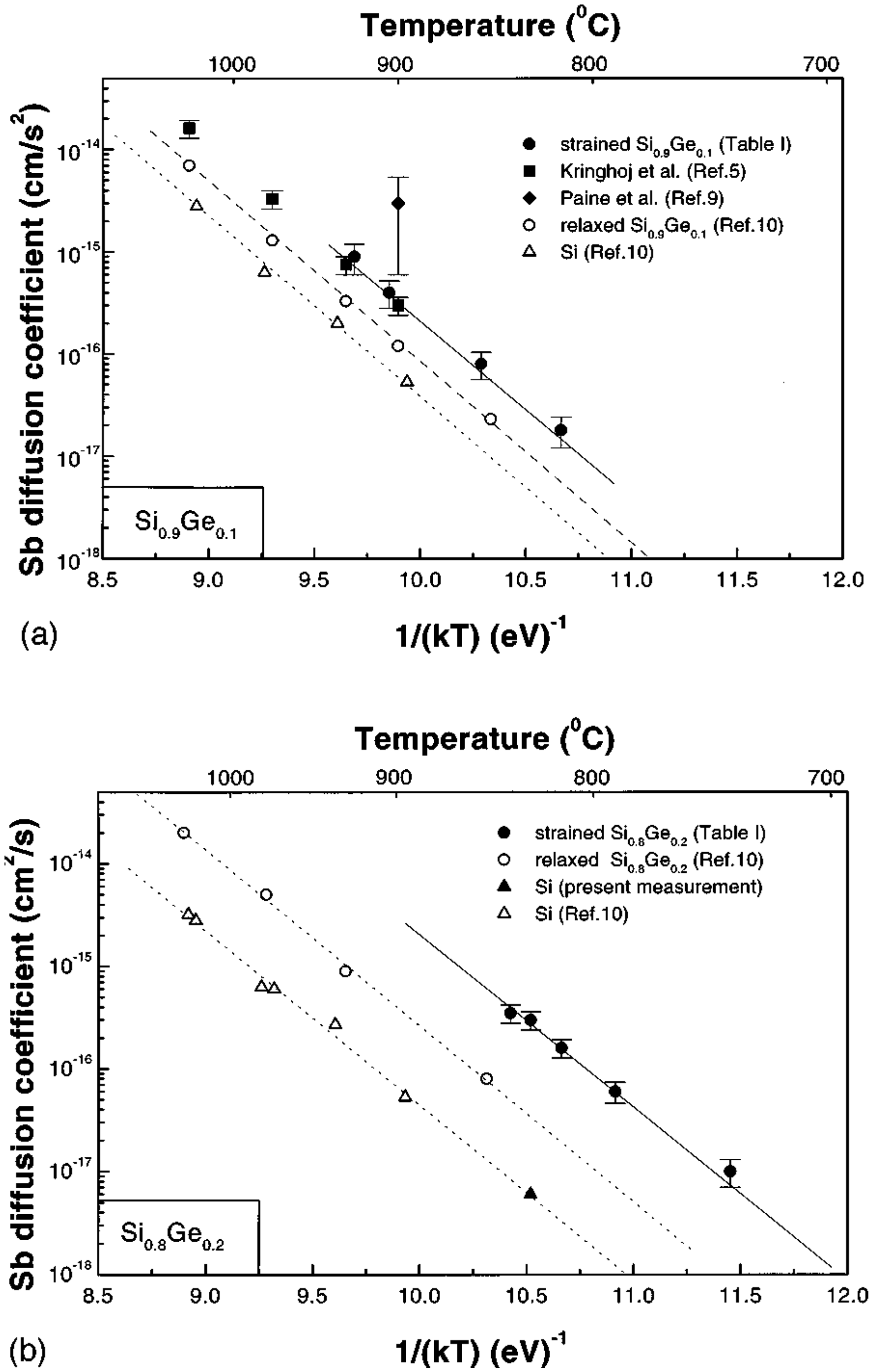


- Also called energy barrier for diffusion

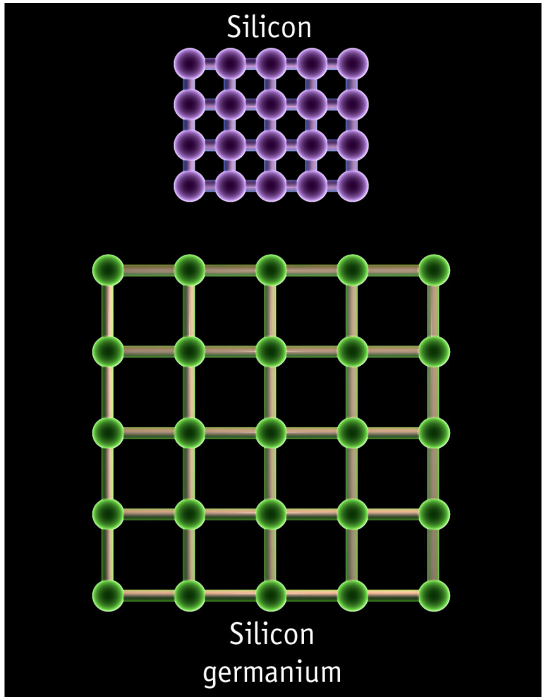
## Lecture 8: Diffusion

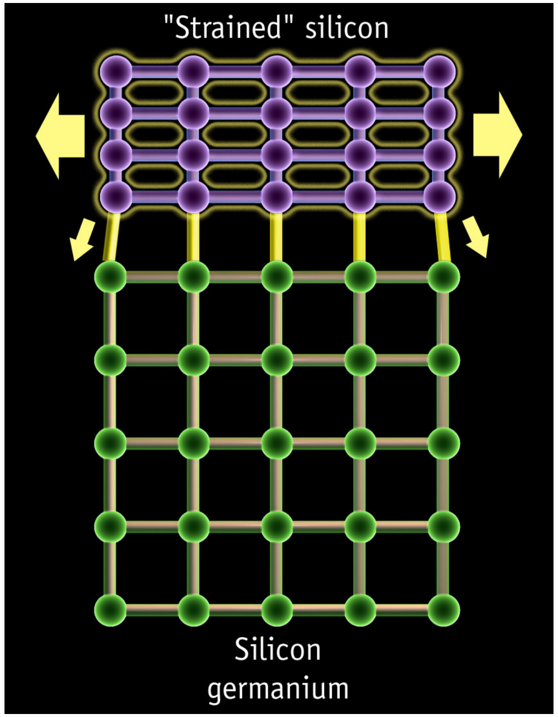
- Phenomenology of diffusion: describing diffusion in terms of diffusion flux
- Microscopic diffusion mechanism
- **Sb diffusion as a function of temperature as stress in Si/SiGe heterostructures**


as deposited
790 °C, 1h
790 °C, 5h
numerical fits
Si0.8Ge0.2
Sb concentration (cm-3)
10^19
10^18
10^17
10^16
0
500
1000
1500
2000
Depth (Å)


Temperature (⁰C)
1000
900
800
700
Sb diffusion coefficient (cm/s²)
10⁻¹⁴
10⁻¹⁵
10⁻¹⁶
10⁻¹⁷
10⁻¹⁸
● strained Si0.9Ge0.1 (Table I)
■ Kringhoj et al. (Ref.5)
◆ Paine et al. (Ref.9)
○ relaxed Si0.9Ge0.1 (Ref.10)
△ Si (Ref.10)
Si0.9Ge0.1
8.5
9.0
9.5
10.0
10.5
11.0
11.5
12.0
(a)
1/(kT) (eV)⁻¹
Temperature (⁰C)
1000
900
800
700
Sb diffusion coefficient (cm²/s)
10⁻¹⁴
10⁻¹⁵
10⁻¹⁶
10⁻¹⁷
10⁻¹⁸
● strained Si0.8Ge0.2 (Table I)
○ relaxed Si0.8Ge0.2 (Ref.10)
▲ Si (present measurement)
△ Si (Ref.10)
Si0.8Ge0.2
8.5
9.0
9.5
10.0
10.5
11.0
11.5
12.0
(b)
1/(kT) (eV)⁻¹

# Strained silicon





- How does it work?
- Basic idea: Change the lattice constant of material